



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:52 PM GMT

PDB ID : 4DPM
Title : Structure of malonyl-coenzyme A reductase from crenarchaeota in complex with CoA
Authors : Demmer, U.; Warkentin, E.; Srivastava, A.; Kockelkorn, D.; Fuchs, G.; Ermler, U.
Deposited on : 2012-02-13
Resolution : 2.30 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

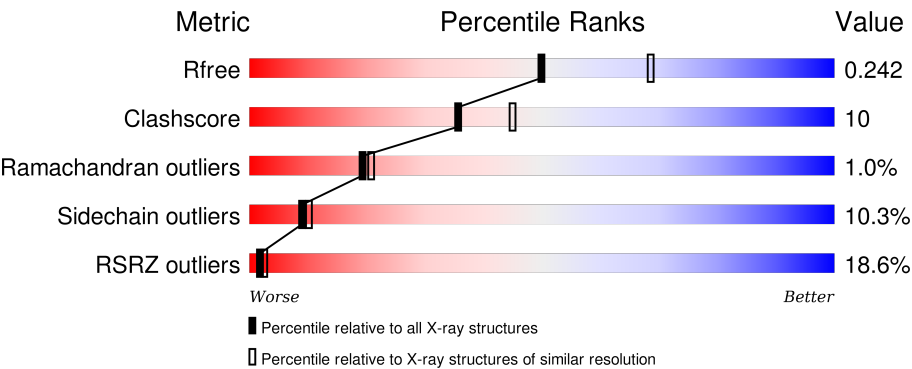
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	359	<div><div>2%</div><div><div></div><div>56%</div><div>35%</div><div>7%</div><div>..</div></div></div>
1	B	359	<div><div>%</div><div><div></div><div>61%</div><div>31%</div><div>5%</div><div>..</div></div></div>
1	C	359	<div><div>18%</div><div><div></div><div>72%</div><div>23%</div><div>..</div></div></div>
1	D	359	<div><div>38%</div><div><div></div><div>73%</div><div>22%</div><div>..</div></div></div>
1	E	359	<div><div>23%</div><div><div></div><div>74%</div><div>20%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	359	<div><div></div><div>28%</div><div></div><div>74%</div><div></div><div>22%</div><div></div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17284 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 Malonyl-CoA/succinyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2743	1759	466	510	8			
1	B	354	Total	C	N	O	S	0	0	0
			2743	1759	466	510	8			
1	C	354	Total	C	N	O	S	0	0	0
			2743	1759	466	510	8			
1	D	354	Total	C	N	O	S	0	0	0
			2743	1759	466	510	8			
1	E	353	Total	C	N	O	S	0	0	0
			2732	1753	462	509	8			
1	F	353	Total	C	N	O	S	0	0	0
			2732	1753	462	509	8			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	E	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	F	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

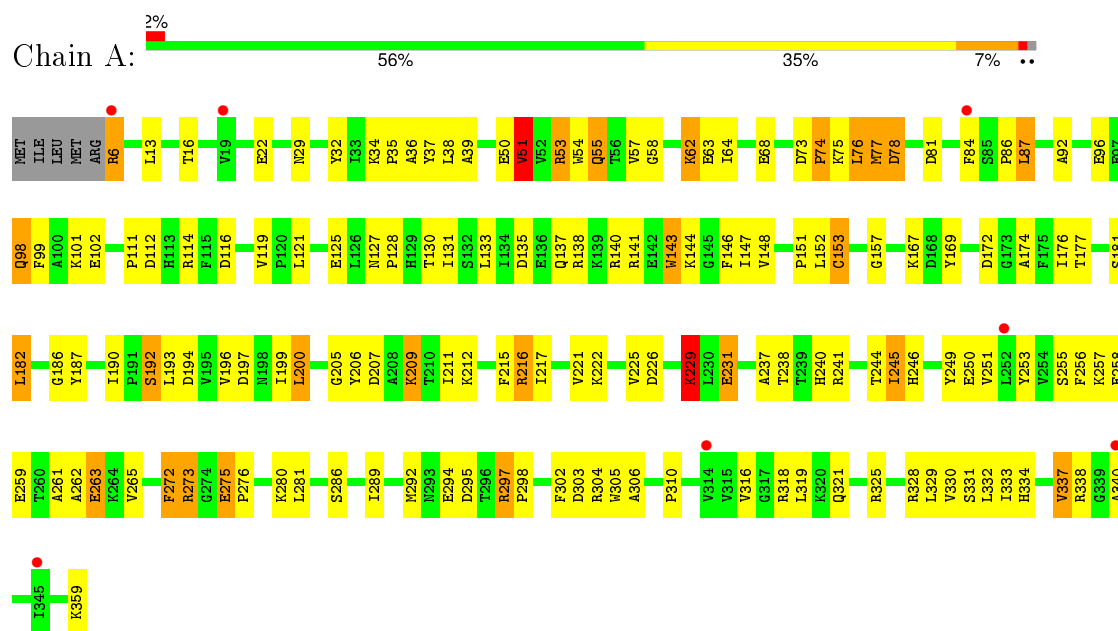
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	184	Total	O	0	0
			184	184		
4	B	172	Total	O	0	0
			172	172		
4	C	59	Total	O	0	0
			59	59		
4	D	57	Total	O	0	0
			57	57		
4	E	52	Total	O	0	0
			52	52		
4	F	30	Total	O	0	0
			30	30		

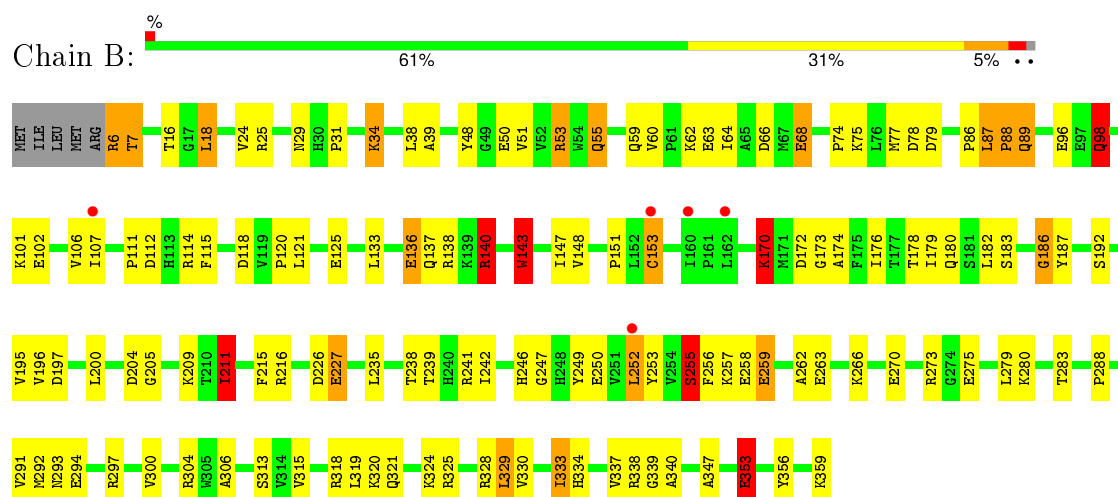
3 Residue-property plots

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

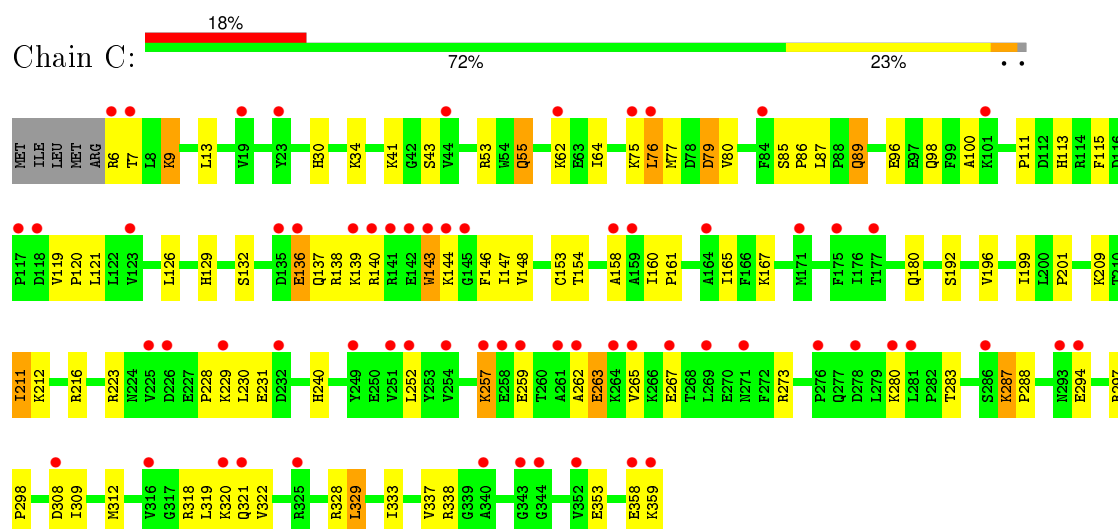
- Molecule 1: Malonyl-CoA/succinyl-CoA reductase



- Molecule 1: Malonyl-CoA/succinyl-CoA reductase



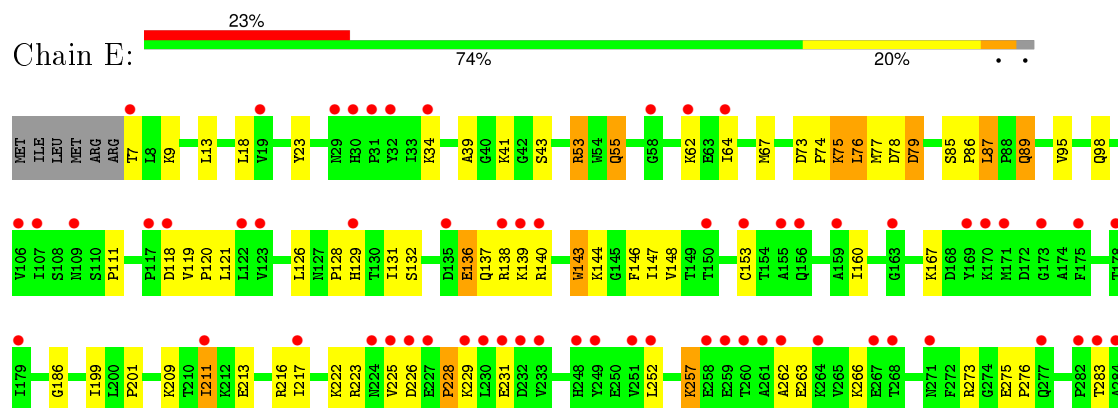
- Molecule 1: Malonyl-CoA/succinyl-CoA reductase

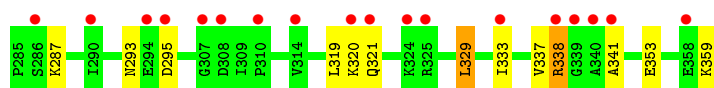


- Molecule 1: Malonyl-CoA/succinyl-CoA reductase

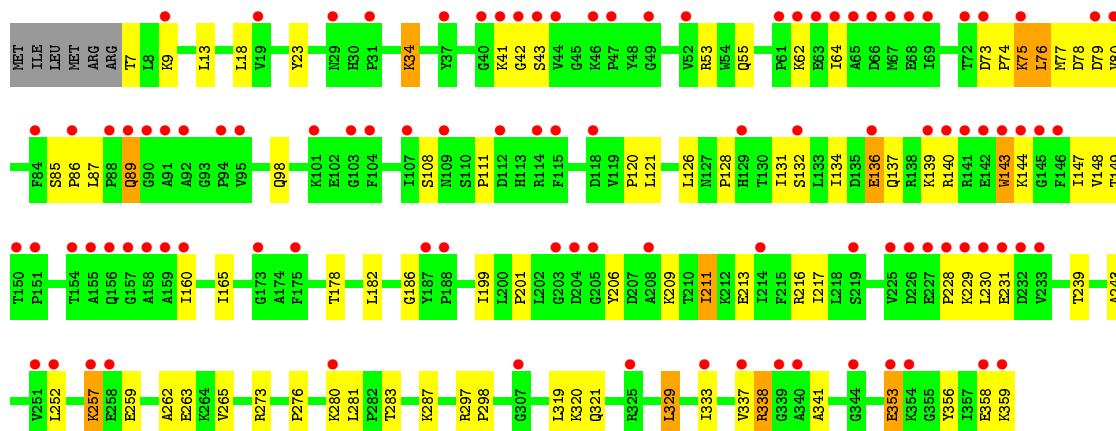


- Molecule 1: Malonyl-CoA/succinyl-CoA reductase





- Molecule 1: Malonyl-CoA/succinyl-CoA reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	111.63Å 137.62Å 362.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.9 (30.00-2.30) 87.9 (29.89-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0095	Depositor
R, R_{free}	0.198 , 0.247 0.195 , 0.242	Depositor DCC
R_{free} test set	6243 reflections (6.06%)	DCC
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 108584 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17284	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: COA, MG

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	2.14	89/2804 (3.2%)	1.64	55/3808 (1.4%)
1	B	2.00	76/2804 (2.7%)	1.53	34/3808 (0.9%)
1	C	0.90	0/2804	0.83	0/3808
1	D	0.76	0/2804	0.76	1/3808 (0.0%)
1	E	0.84	0/2793	0.82	2/3794 (0.1%)
1	F	0.70	0/2793	0.75	1/3794 (0.0%)
All	All	1.36	165/16802 (1.0%)	1.12	93/22820 (0.4%)

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	0	1

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	353	GLU	CB-CG	14.56	1.79	1.52
1	A	302	PHE	CE1-CZ	12.24	1.60	1.37
1	A	255	SER	CB-OG	-11.06	1.27	1.42
1	A	53	ARG	CG-CD	10.35	1.77	1.51
1	A	187	TYR	CD2-CE2	10.24	1.54	1.39
1	B	255	SER	CB-OG	-9.96	1.29	1.42
1	B	187	TYR	CD2-CE2	9.37	1.53	1.39
1	A	200	LEU	CG-CD1	8.98	1.85	1.51
1	B	275	GLU	CD-OE2	8.90	1.35	1.25
1	B	353	GLU	CG-CD	-8.83	1.38	1.51
1	B	53	ARG	CG-CD	8.61	1.73	1.51
1	A	192	SER	C-O	8.54	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	ASP	CB-CG	8.49	1.69	1.51
1	B	29	ASN	CB-CG	8.32	1.70	1.51
1	B	300	VAL	CB-CG2	8.26	1.70	1.52
1	B	215	PHE	CG-CD1	8.05	1.50	1.38
1	A	241	ARG	CZ-NH1	8.03	1.43	1.33
1	A	51	VAL	CB-CG1	-7.93	1.36	1.52
1	B	115	PHE	CE2-CZ	7.68	1.51	1.37
1	B	253	TYR	CE1-CZ	7.61	1.48	1.38
1	B	39	ALA	CA-CB	-7.59	1.36	1.52
1	A	302	PHE	CG-CD2	7.59	1.50	1.38
1	A	32	TYR	CD2-CE2	-7.54	1.28	1.39
1	B	88	PRO	CG-CD	7.49	1.75	1.50
1	A	205	GLY	N-CA	7.49	1.57	1.46
1	B	170	LYS	CD-CE	7.42	1.69	1.51
1	B	153	CYS	CB-SG	7.40	1.94	1.82
1	B	241	ARG	CZ-NH1	7.39	1.42	1.33
1	B	192	SER	CB-OG	7.38	1.51	1.42
1	B	294	GLU	CG-CD	7.35	1.62	1.51
1	A	54	TRP	CE3-CZ3	7.33	1.50	1.38
1	A	206	TYR	CG-CD1	7.28	1.48	1.39
1	A	249	TYR	CD2-CE2	-7.11	1.28	1.39
1	B	183	SER	CA-CB	7.09	1.63	1.52
1	B	118	ASP	CB-CG	6.97	1.66	1.51
1	B	328	ARG	CG-CD	6.96	1.69	1.51
1	A	114	ARG	CZ-NH1	6.95	1.42	1.33
1	A	310	PRO	N-CA	6.93	1.59	1.47
1	B	115	PHE	CG-CD2	6.91	1.49	1.38
1	A	229	LYS	CD-CE	6.90	1.68	1.51
1	B	98	GLN	CG-CD	6.90	1.67	1.51
1	A	38	LEU	N-CA	6.86	1.60	1.46
1	A	68	GLU	CG-CD	6.82	1.62	1.51
1	B	115	PHE	CD1-CE1	6.81	1.52	1.39
1	B	215	PHE	CE2-CZ	6.81	1.50	1.37
1	B	304	ARG	CB-CG	6.78	1.70	1.52
1	A	329	LEU	C-O	6.74	1.36	1.23
1	A	99	PHE	CD1-CE1	6.73	1.52	1.39
1	A	246	HIS	C-O	6.68	1.36	1.23
1	A	306	ALA	CA-CB	6.67	1.66	1.52
1	A	146	PHE	CE1-CZ	6.67	1.50	1.37
1	A	148	VAL	CB-CG2	6.66	1.66	1.52
1	B	174	ALA	CA-CB	6.64	1.66	1.52
1	B	136	GLU	CG-CD	6.62	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	186	GLY	C-O	6.57	1.34	1.23
1	B	275	GLU	CG-CD	6.56	1.61	1.51
1	A	221	VAL	CB-CG2	-6.52	1.39	1.52
1	A	35	PRO	CG-CD	6.46	1.72	1.50
1	A	294	GLU	CG-CD	6.45	1.61	1.51
1	A	286	SER	CB-OG	-6.44	1.33	1.42
1	A	186	GLY	C-O	6.43	1.33	1.23
1	A	263	GLU	CG-CD	6.40	1.61	1.51
1	B	313	SER	CB-OG	-6.39	1.33	1.42
1	A	328	ARG	CZ-NH1	6.39	1.41	1.33
1	A	111	PRO	CA-CB	6.35	1.66	1.53
1	B	253	TYR	CG-CD2	6.30	1.47	1.39
1	A	225	VAL	CB-CG2	6.25	1.66	1.52
1	A	256	PHE	CE2-CZ	6.23	1.49	1.37
1	B	263	GLU	CG-CD	6.21	1.61	1.51
1	A	174	ALA	CA-CB	6.20	1.65	1.52
1	A	258	GLU	CD-OE2	6.20	1.32	1.25
1	A	245	ILE	C-O	6.19	1.35	1.23
1	A	212	LYS	CD-CE	6.16	1.66	1.51
1	B	25	ARG	NE-CZ	6.13	1.41	1.33
1	A	207	ASP	CB-CG	6.11	1.64	1.51
1	A	275	GLU	CB-CG	-6.10	1.40	1.52
1	B	96	GLU	CD-OE1	6.06	1.32	1.25
1	B	339	GLY	C-O	6.04	1.33	1.23
1	A	157	GLY	N-CA	6.02	1.55	1.46
1	A	187	TYR	C-O	-6.01	1.11	1.23
1	B	258	GLU	CG-CD	6.00	1.60	1.51
1	A	157	GLY	C-O	5.99	1.33	1.23
1	A	197	ASP	CG-OD2	5.96	1.39	1.25
1	B	249	TYR	CG-CD1	5.89	1.46	1.39
1	A	272	PHE	CE1-CZ	5.88	1.48	1.37
1	A	125	GLU	CD-OE1	5.87	1.32	1.25
1	B	204	ASP	C-O	5.84	1.34	1.23
1	B	259	GLU	CD-OE1	5.83	1.32	1.25
1	A	99	PHE	CG-CD2	5.81	1.47	1.38
1	B	297	ARG	CZ-NH1	5.81	1.40	1.33
1	A	297	ARG	CG-CD	5.78	1.66	1.51
1	B	25	ARG	CZ-NH2	5.75	1.40	1.33
1	A	22	GLU	CD-OE1	5.73	1.31	1.25
1	B	246	HIS	C-O	5.72	1.34	1.23
1	B	263	GLU	CB-CG	5.70	1.62	1.52
1	A	238	THR	CB-CG2	5.69	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	GLU	CD-OE2	5.63	1.31	1.25
1	A	240	HIS	C-O	5.61	1.34	1.23
1	B	31	PRO	CG-CD	5.61	1.69	1.50
1	B	353	GLU	CD-OE2	5.60	1.31	1.25
1	A	338	ARG	C-O	5.60	1.33	1.23
1	B	273	ARG	CG-CD	5.59	1.66	1.51
1	A	215	PHE	CE2-CZ	5.58	1.48	1.37
1	A	63	GLU	CG-CD	5.57	1.60	1.51
1	A	37	TYR	CE1-CZ	5.56	1.45	1.38
1	A	256	PHE	CG-CD2	5.56	1.47	1.38
1	A	112	ASP	C-O	5.54	1.33	1.23
1	A	192	SER	CB-OG	5.54	1.49	1.42
1	B	249	TYR	CA-CB	-5.53	1.41	1.53
1	B	34	LYS	CE-NZ	5.52	1.62	1.49
1	B	63	GLU	CG-CD	5.51	1.60	1.51
1	B	330	VAL	CB-CG1	5.51	1.64	1.52
1	A	169	TYR	CE1-CZ	5.50	1.45	1.38
1	A	275	GLU	CG-CD	5.50	1.60	1.51
1	B	347	ALA	CA-CB	5.50	1.64	1.52
1	B	256	PHE	CE1-CZ	5.48	1.47	1.37
1	A	249	TYR	CZ-OH	5.48	1.47	1.37
1	A	250	GLU	CA-CB	-5.47	1.42	1.53
1	B	294	GLU	CD-OE1	5.47	1.31	1.25
1	A	330	VAL	C-O	5.46	1.33	1.23
1	A	63	GLU	CD-OE1	5.46	1.31	1.25
1	B	106	VAL	CB-CG1	5.45	1.64	1.52
1	A	130	THR	CA-CB	5.44	1.67	1.53
1	B	318	ARG	NE-CZ	5.44	1.40	1.33
1	A	333	ILE	C-O	5.43	1.33	1.23
1	B	176	ILE	CB-CG2	-5.42	1.36	1.52
1	A	258	GLU	CD-OE1	5.42	1.31	1.25
1	A	304	ARG	NE-CZ	5.40	1.40	1.33
1	A	63	GLU	CB-CG	5.36	1.62	1.52
1	B	333	ILE	C-O	5.34	1.33	1.23
1	A	330	VAL	CB-CG1	5.32	1.64	1.52
1	A	211	ILE	CA-CB	5.31	1.67	1.54
1	B	197	ASP	CG-OD2	5.30	1.37	1.25
1	A	199	ILE	CA-CB	-5.30	1.42	1.54
1	A	36	ALA	CA-CB	5.30	1.63	1.52
1	B	238	THR	N-CA	-5.29	1.35	1.46
1	B	59	GLN	CB-CG	5.27	1.66	1.52
1	A	238	THR	CA-C	-5.27	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	GLU	CD-OE1	5.26	1.31	1.25
1	B	315	VAL	CB-CG2	5.25	1.63	1.52
1	B	340	ALA	CA-CB	5.24	1.63	1.52
1	B	356	TYR	CE1-CZ	5.23	1.45	1.38
1	B	215	PHE	CD1-CE1	5.22	1.49	1.39
1	A	305	TRP	CG-CD1	5.22	1.44	1.36
1	B	18	LEU	C-O	5.20	1.33	1.23
1	B	247	GLY	CA-C	5.20	1.60	1.51
1	B	280	LYS	CE-NZ	5.20	1.62	1.49
1	A	318	ARG	NE-CZ	5.19	1.39	1.33
1	A	259	GLU	CD-OE1	5.17	1.31	1.25
1	B	306	ALA	CA-CB	5.17	1.63	1.52
1	A	98	GLN	CG-CD	5.17	1.62	1.51
1	B	241	ARG	C-O	5.16	1.33	1.23
1	A	207	ASP	CG-OD1	5.16	1.37	1.25
1	A	176	ILE	N-CA	5.13	1.56	1.46
1	A	253	TYR	CE2-CZ	-5.10	1.31	1.38
1	A	187	TYR	CG-CD1	5.09	1.45	1.39
1	A	197	ASP	CG-OD1	5.09	1.37	1.25
1	B	136	GLU	CD-OE1	5.08	1.31	1.25
1	B	215	PHE	CD2-CE2	5.07	1.49	1.39
1	A	84	PHE	CE2-CZ	5.05	1.47	1.37
1	B	205	GLY	C-O	5.05	1.31	1.23
1	A	333	ILE	CA-C	5.04	1.66	1.52
1	B	143	TRP	CE3-CZ3	5.04	1.47	1.38
1	B	88	PRO	CA-CB	5.04	1.63	1.53
1	B	227	GLU	CB-CG	5.03	1.61	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH2	-15.06	112.77	120.30
1	B	328	ARG	NE-CZ-NH2	13.87	127.23	120.30
1	A	255	SER	N-CA-CB	-11.24	93.64	110.50
1	A	141	ARG	NE-CZ-NH2	-11.07	114.77	120.30
1	B	318	ARG	NE-CZ-NH1	10.37	125.49	120.30
1	B	200	LEU	CB-CG-CD2	-9.66	94.58	111.00
1	B	114	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	A	114	ARG	NE-CZ-NH1	9.09	124.85	120.30
1	A	78	ASP	CB-CG-OD1	-8.80	110.38	118.30
1	A	328	ARG	NE-CZ-NH1	-8.63	115.99	120.30
1	A	141	ARG	NE-CZ-NH1	8.47	124.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	MET	CG-SD-CE	-8.46	86.67	100.20
1	B	292	MET	CG-SD-CE	-7.93	87.51	100.20
1	B	140	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	B	329	LEU	CA-CB-CG	7.86	133.38	115.30
1	B	353	GLU	CG-CD-OE1	-7.84	102.61	118.30
1	B	252	LEU	CB-CG-CD2	-7.82	97.71	111.00
1	A	319	LEU	CB-CG-CD1	7.39	123.56	111.00
1	A	295	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	78	ASP	CB-CG-OD2	7.07	124.67	118.30
1	A	194	ASP	CB-CG-OD2	6.91	124.52	118.30
1	B	77	MET	CG-SD-CE	-6.84	89.26	100.20
1	B	209	LYS	CD-CE-NZ	6.75	127.23	111.70
1	A	245	ILE	CG1-CB-CG2	-6.71	96.64	111.40
1	A	77	MET	CG-SD-CE	-6.69	89.49	100.20
1	A	216	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	255	SER	N-CA-CB	-6.63	100.55	110.50
1	B	216	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	303	ASP	CB-CG-OD2	6.55	124.20	118.30
1	A	133	LEU	CB-CG-CD1	-6.51	99.92	111.00
1	A	76	LEU	CA-CB-CG	6.49	130.23	115.30
1	B	319	LEU	CB-CG-CD2	-6.41	100.11	111.00
1	B	211	ILE	CA-CB-CG2	6.36	123.61	110.90
1	B	250	GLU	OE1-CD-OE2	-6.24	115.82	123.30
1	A	241	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	107	ILE	CG1-CB-CG2	-6.15	97.86	111.40
1	B	133	LEU	CB-CG-CD1	-6.15	100.55	111.00
1	B	297	ARG	CD-NE-CZ	-6.14	115.00	123.60
1	A	196	VAL	CA-CB-CG2	-6.13	101.71	110.90
1	B	114	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	207	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	87	LEU	CB-CG-CD1	6.05	121.29	111.00
1	A	289	ILE	CG1-CB-CG2	-6.04	98.12	111.40
1	A	216	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	200	LEU	CB-CA-C	-6.00	98.80	110.20
1	A	211	ILE	CA-CB-CG2	5.98	122.85	110.90
1	A	182	LEU	CB-CG-CD2	-5.96	100.86	111.00
1	B	87	LEU	CB-CG-CD1	5.96	121.13	111.00
1	B	195	VAL	CB-CA-C	-5.81	100.36	111.40
1	A	212	LYS	CD-CE-NZ	-5.80	98.35	111.70
1	B	250	GLU	CG-CD-OE2	5.76	129.83	118.30
1	A	251	VAL	CG1-CB-CG2	-5.73	101.74	110.90
1	B	66	ASP	CB-CG-OD1	5.72	123.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	138	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	148	VAL	CG1-CB-CG2	-5.62	101.90	110.90
1	A	328	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	B	89	GLN	CB-CA-C	-5.57	99.26	110.40
1	A	216	ARG	CD-NE-CZ	5.56	131.38	123.60
1	B	138	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	204	ASP	CB-CG-OD1	5.52	123.26	118.30
1	A	257	LYS	CB-CA-C	-5.50	99.39	110.40
1	A	194	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	167	LYS	CD-CE-NZ	-5.49	99.07	111.70
1	A	281	LEU	CB-CG-CD1	-5.49	101.67	111.00
1	A	338	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	138	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	81	ASP	CB-CG-OD1	5.43	123.18	118.30
1	A	135	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	353	GLU	CB-CG-CD	-5.37	99.71	114.20
1	A	273	ARG	CB-CA-C	-5.35	99.70	110.40
1	B	353	GLU	OE1-CD-OE2	5.35	129.72	123.30
1	A	193	LEU	CB-CG-CD1	5.33	120.07	111.00
1	A	177	THR	N-CA-CB	-5.33	100.17	110.30
1	A	265	VAL	CG1-CB-CG2	-5.29	102.44	110.90
1	A	273	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	A	211	ILE	N-CA-C	-5.24	96.85	111.00
1	B	18	LEU	CA-CB-CG	-5.19	103.36	115.30
1	A	325	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	292	MET	CB-CG-SD	-5.18	96.86	112.40
1	B	178	THR	CA-CB-CG2	5.17	119.64	112.40
1	D	273	ARG	CG-CD-NE	5.16	122.63	111.80
1	A	190	ILE	CG1-CB-CG2	-5.15	100.07	111.40
1	F	338	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	205	GLY	N-CA-C	-5.11	100.33	113.10
1	B	101	LYS	CD-CE-NZ	-5.09	100.00	111.70
1	A	112	ASP	CB-CG-OD1	5.08	122.87	118.30
1	E	338	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	211	ILE	N-CA-CB	-5.06	99.15	110.80
1	A	332	LEU	CB-CG-CD2	5.06	119.61	111.00
1	A	172	ASP	CB-CG-OD1	5.04	122.83	118.30
1	E	53	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	279	LEU	CB-CG-CD1	5.01	119.51	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ALA	Mainchain

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	2743	0	2799	55	0
1	B	2743	0	2799	56	0
1	C	2743	0	2799	63	1
1	D	2743	0	2799	50	0
1	E	2732	0	2786	53	0
1	F	2732	0	2786	44	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	48	0	32	1	0
3	B	48	0	32	3	0
3	C	48	0	32	1	0
3	D	48	0	32	4	0
3	E	48	0	32	1	0
3	F	48	0	32	2	0
4	A	184	0	0	13	0
4	B	172	0	0	5	0
4	C	59	0	0	20	0
4	D	57	0	0	14	0
4	E	52	0	0	10	0
4	F	30	0	0	12	0
All	All	17284	0	16960	326	1

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 (326) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ARG:CD	1:A:53:ARG:CG	1.77	1.61
1:B:353:GLU:CG	1:B:353:GLU:CB	1.79	1.58
1:A:200:LEU:CG	1:A:200:LEU:CD1	1.85	1.54
1:B:88:PRO:CD	1:B:88:PRO:CG	1.75	1.51
1:C:223:ARG:HA	4:C:656:HOH:O	1.19	1.29
1:F:134:ILE:HG22	4:F:613:HOH:O	1.22	1.28
1:A:231:GLU:HG3	4:A:733:HOH:O	1.41	1.16
1:E:223:ARG:HA	4:E:643:HOH:O	1.41	1.15
1:C:100:ALA:HB2	4:C:655:HOH:O	1.54	1.07
1:F:34:LYS:HG2	4:F:628:HOH:O	1.52	1.06
1:B:353:GLU:HB2	1:B:353:GLU:OE1	1.60	1.02
1:A:262:ALA:H	1:A:321:GLN:HE22	1.07	1.00
1:C:6:ARG:NH1	1:C:6:ARG:HA	1.77	0.99
1:B:353:GLU:OE1	1:B:353:GLU:CB	2.10	0.98
1:C:6:ARG:HH11	1:C:6:ARG:HA	1.28	0.94
1:C:267:GLU:HG3	4:C:650:HOH:O	1.67	0.93
1:F:206:TYR:HA	4:F:627:HOH:O	1.70	0.89
1:C:13:LEU:HD12	1:C:85:SER:HB2	1.57	0.86
1:B:353:GLU:CD	1:B:353:GLU:CB	2.44	0.85
1:E:252:LEU:HB2	1:E:329:LEU:CD2	2.06	0.85
1:B:353:GLU:C	1:B:353:GLU:HG3	1.95	0.84
1:A:262:ALA:H	1:A:321:GLN:NE2	1.75	0.84
1:C:252:LEU:HB2	1:C:329:LEU:CD2	2.08	0.84
1:B:68:GLU:HG2	4:B:741:HOH:O	1.80	0.81
1:C:167:LYS:HA	4:C:656:HOH:O	1.81	0.81
1:A:137:GLN:HE22	1:A:147:ILE:H	1.26	0.81
1:F:34:LYS:CG	4:F:628:HOH:O	2.18	0.80
1:D:353:GLU:HA	4:D:654:HOH:O	1.81	0.80
1:C:294:GLU:HB3	4:C:638:HOH:O	1.82	0.80
1:B:353:GLU:C	1:B:353:GLU:CG	2.49	0.79
1:C:137:GLN:HE21	1:C:143:TRP:HE1	1.31	0.79
1:F:252:LEU:HB2	1:F:329:LEU:CD2	2.13	0.79
1:B:6:ARG:HD2	1:B:7:THR:N	1.98	0.78
1:B:6:ARG:CD	1:B:7:THR:H	1.96	0.78
1:D:252:LEU:HB2	1:D:329:LEU:CD2	2.12	0.78
1:B:137:GLN:HE22	1:B:147:ILE:H	1.32	0.77
1:D:6:ARG:HH11	1:D:6:ARG:N	1.83	0.76
1:C:252:LEU:HB2	1:C:329:LEU:HD23	1.67	0.75
1:D:262:ALA:H	1:D:321:GLN:HE22	1.33	0.74
1:A:53:ARG:CD	1:A:53:ARG:CB	2.65	0.73
1:D:230:LEU:HD23	4:D:611:HOH:O	1.87	0.73
1:E:129:HIS:CD2	1:E:222:LYS:HZ1	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ARG:NE	1:A:53:ARG:CG	2.51	0.73
1:B:353:GLU:CG	1:B:353:GLU:CA	2.67	0.72
1:A:6:ARG:CZ	1:A:6:ARG:HB3	2.20	0.71
1:B:53:ARG:HE	1:B:55:GLN:NE2	1.89	0.71
1:C:294:GLU:HA	4:C:618:HOH:O	1.92	0.70
1:C:120:PRO:HA	4:C:643:HOH:O	1.91	0.69
1:B:353:GLU:HG3	1:B:353:GLU:O	1.91	0.69
1:B:6:ARG:HD2	1:B:7:THR:H	1.53	0.69
1:A:262:ALA:N	1:A:321:GLN:HE22	1.86	0.69
1:E:252:LEU:HB2	1:E:329:LEU:HD23	1.73	0.68
1:D:352:VAL:HG12	4:D:654:HOH:O	1.94	0.68
1:C:89:GLN:HG2	1:C:111:PRO:HG2	1.76	0.68
1:F:137:GLN:HE21	1:F:143:TRP:HE1	1.40	0.68
1:C:100:ALA:CA	4:C:655:HOH:O	2.42	0.68
1:E:167:LYS:HA	4:E:643:HOH:O	1.92	0.67
1:A:53:ARG:HH21	1:A:55:GLN:HE22	1.39	0.67
1:F:252:LEU:HB2	1:F:329:LEU:HD23	1.76	0.67
1:E:225:VAL:HG22	4:E:649:HOH:O	1.94	0.66
1:E:226:ASP:HB2	4:E:608:HOH:O	1.96	0.66
1:A:53:ARG:HD2	4:A:707:HOH:O	1.96	0.66
1:E:223:ARG:HB2	4:E:646:HOH:O	1.95	0.66
1:C:262:ALA:H	1:C:321:GLN:HE22	1.41	0.66
1:E:262:ALA:H	1:E:321:GLN:HE22	1.42	0.66
1:A:53:ARG:HB2	4:A:707:HOH:O	1.95	0.65
1:B:6:ARG:NH1	4:B:768:HOH:O	2.30	0.65
1:A:229:LYS:N	1:A:229:LYS:HD3	2.12	0.65
1:F:120:PRO:HG2	1:F:148:VAL:HG22	1.77	0.65
1:E:89:GLN:HG2	1:E:111:PRO:HG2	1.79	0.65
1:C:153:CYS:HG	3:C:402:COA:HS1	0.69	0.65
1:B:137:GLN:HE21	1:B:143:TRP:HE1	1.41	0.65
1:E:129:HIS:CD2	1:E:222:LYS:NZ	2.65	0.64
3:E:402:COA:O5P	3:E:402:COA:H22	1.98	0.64
1:B:18:LEU:HD12	1:B:186:GLY:HA2	1.81	0.63
1:E:295:ASP:OD2	4:E:645:HOH:O	2.15	0.63
1:D:137:GLN:HE21	1:D:143:TRP:HE1	1.46	0.63
1:B:262:ALA:H	1:B:321:GLN:HE22	1.45	0.62
1:A:226:ASP:HB2	4:A:776:HOH:O	1.98	0.62
1:C:129:HIS:ND1	4:C:601:HOH:O	2.31	0.62
1:A:200:LEU:CD2	1:A:200:LEU:CD1	2.78	0.62
1:C:13:LEU:HD12	1:C:85:SER:CB	2.29	0.62
1:F:18:LEU:HD12	1:F:186:GLY:HA2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:PRO:HG2	1:C:148:VAL:HG22	1.82	0.61
1:F:262:ALA:H	1:F:321:GLN:HE22	1.46	0.61
1:E:137:GLN:HE21	1:E:143:TRP:HE1	1.48	0.61
1:F:42:GLY:CA	4:F:624:HOH:O	2.47	0.61
1:B:153:CYS:SG	3:B:402:COA:S1P	2.97	0.61
1:F:42:GLY:N	4:F:624:HOH:O	2.34	0.61
1:D:120:PRO:HG2	1:D:148:VAL:HG22	1.80	0.61
1:D:252:LEU:HB2	1:D:329:LEU:HD23	1.82	0.60
1:C:318:ARG:HA	4:C:602:HOH:O	2.00	0.60
1:C:267:GLU:CA	4:C:650:HOH:O	2.49	0.60
1:D:135:ASP:HA	4:D:610:HOH:O	2.01	0.60
1:C:228:PRO:HG3	1:C:257:LYS:HD2	1.84	0.60
1:D:262:ALA:H	1:D:321:GLN:NE2	1.99	0.60
1:A:272:PHE:O	1:A:273:ARG:NH1	2.35	0.60
3:B:402:COA:H10	4:B:743:HOH:O	2.01	0.60
1:A:92:ALA:O	1:A:96:GLU:HG3	2.02	0.59
1:D:143:TRP:HA	4:D:645:HOH:O	2.01	0.59
1:B:259:GLU:HG3	1:B:324:LYS:HB3	1.83	0.59
1:A:74:PRO:HB3	1:A:102:GLU:HG3	1.85	0.59
1:B:120:PRO:HG2	1:B:148:VAL:HG22	1.83	0.59
1:A:16:THR:HG21	1:A:51:VAL:HG22	1.85	0.58
1:D:70:LYS:HG2	4:D:607:HOH:O	2.03	0.57
1:A:6:ARG:CZ	1:A:6:ARG:CB	2.81	0.57
1:C:267:GLU:N	4:C:650:HOH:O	2.36	0.57
1:A:151:PRO:CG	1:A:217:ILE:HD11	2.34	0.57
1:D:126:LEU:HD11	1:D:160:ILE:HA	1.86	0.57
1:C:138:ARG:HH21	1:C:146:PHE:HD2	1.52	0.57
1:A:200:LEU:CD1	1:A:200:LEU:CB	2.77	0.57
1:E:120:PRO:HG2	1:E:148:VAL:HG22	1.86	0.56
1:B:24:VAL:HG13	1:B:64:ILE:HG13	1.87	0.56
1:B:74:PRO:HB2	1:B:102:GLU:HG3	1.86	0.56
1:C:137:GLN:NE2	1:C:143:TRP:HE1	2.00	0.56
1:A:50:GLU:OE1	4:A:772:HOH:O	2.18	0.56
1:E:67:MET:HE3	4:E:614:HOH:O	2.04	0.56
1:D:228:PRO:HG3	1:D:257:LYS:HD2	1.89	0.55
1:C:89:GLN:CG	1:C:111:PRO:HG2	2.37	0.55
1:B:137:GLN:HE22	1:B:147:ILE:N	2.04	0.55
1:C:53:ARG:HG3	1:C:53:ARG:HH11	1.72	0.55
1:D:137:GLN:HE22	1:D:147:ILE:H	1.56	0.54
1:F:131:ILE:C	4:F:629:HOH:O	2.46	0.54
1:F:132:SER:N	4:F:629:HOH:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ILE:HD11	1:B:196:VAL:HG12	1.88	0.54
1:E:228:PRO:HG3	1:E:257:LYS:HD2	1.90	0.54
1:D:75:LYS:HE3	4:D:656:HOH:O	2.07	0.53
1:C:262:ALA:H	1:C:321:GLN:NE2	2.03	0.53
1:F:262:ALA:H	1:F:321:GLN:NE2	2.06	0.53
1:E:121:LEU:HD23	1:E:216:ARG:HG2	1.89	0.53
1:A:6:ARG:N	4:A:684:HOH:O	2.41	0.53
1:B:16:THR:HG21	1:B:51:VAL:HG22	1.90	0.53
1:B:60:VAL:HG23	4:B:716:HOH:O	2.08	0.53
1:A:127:ASN:N	1:A:128:PRO:CD	2.71	0.53
1:F:228:PRO:HG3	1:F:257:LYS:HD2	1.91	0.52
1:E:262:ALA:H	1:E:321:GLN:NE2	2.08	0.52
1:D:77:MET:O	1:D:80:VAL:N	2.37	0.52
1:E:283:THR:HG22	1:E:283:THR:O	2.10	0.52
1:B:6:ARG:CD	1:B:7:THR:N	2.65	0.52
1:C:154:THR:HG21	1:C:180:GLN:NE2	2.25	0.52
1:E:167:LYS:HG3	4:E:643:HOH:O	2.09	0.52
1:F:206:TYR:CA	4:F:627:HOH:O	2.42	0.52
1:F:132:SER:HA	4:F:629:HOH:O	2.09	0.52
1:D:27:LEU:HD21	1:D:345:ILE:HG12	1.92	0.52
1:D:213:GLU:O	1:D:217:ILE:HG13	2.10	0.51
1:F:128:PRO:O	1:F:131:ILE:HG12	2.11	0.51
1:D:18:LEU:HD12	1:D:186:GLY:HA2	1.92	0.51
1:E:126:LEU:HD11	1:E:160:ILE:HA	1.93	0.51
1:D:202:LEU:HD22	4:D:634:HOH:O	2.11	0.51
1:E:118:ASP:HA	4:E:644:HOH:O	2.10	0.51
1:C:121:LEU:HD23	1:C:216:ARG:HG2	1.92	0.51
1:E:53:ARG:HE	1:E:55:GLN:NE2	2.09	0.51
1:C:119:VAL:O	1:C:216:ARG:NH2	2.42	0.50
1:D:280:LYS:HB3	4:D:652:HOH:O	2.11	0.50
1:D:38:LEU:O	4:D:651:HOH:O	2.18	0.50
1:C:136:GLU:O	1:C:140:ARG:HB2	2.11	0.50
1:B:334:HIS:CE1	1:B:337:VAL:HG23	2.46	0.50
1:D:13:LEU:HD12	1:D:85:SER:HB2	1.94	0.50
1:B:53:ARG:NE	1:B:55:GLN:NE2	2.59	0.49
1:E:89:GLN:CG	1:E:111:PRO:HG2	2.42	0.49
1:B:266:LYS:NZ	1:B:293:ASN:ND2	2.59	0.49
1:B:53:ARG:HH21	1:B:55:GLN:HE22	1.60	0.49
1:B:262:ALA:H	1:B:321:GLN:NE2	2.10	0.49
1:B:125:GLU:N	1:B:125:GLU:OE1	2.44	0.49
1:A:137:GLN:HE21	1:A:143:TRP:HE1	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:333:ILE:HD11	1:F:338:ARG:HG3	1.94	0.49
1:B:136:GLU:O	1:B:140:ARG:HG3	2.12	0.49
1:D:127:ASN:HB2	1:D:130:THR:HG23	1.94	0.49
1:A:76:LEU:HD13	4:A:769:HOH:O	2.13	0.49
1:E:18:LEU:HD12	1:E:186:GLY:HA2	1.95	0.49
1:A:98:GLN:HG2	4:A:710:HOH:O	2.13	0.49
1:C:77:MET:O	1:C:80:VAL:N	2.42	0.49
1:F:53:ARG:HG3	4:F:622:HOH:O	2.13	0.48
1:C:100:ALA:CB	4:C:655:HOH:O	2.24	0.48
1:B:53:ARG:HE	1:B:55:GLN:HE21	1.60	0.48
1:E:137:GLN:HE22	1:E:147:ILE:H	1.61	0.48
1:D:153:CYS:SG	3:D:402:COA:S1P	3.05	0.48
1:B:288:PRO:HD2	4:B:629:HOH:O	2.12	0.48
1:A:73:ASP:H	1:A:77:MET:CE	2.26	0.48
1:C:115:PHE:CZ	1:C:212:LYS:HD3	2.48	0.48
1:A:359:LYS:HE2	4:A:730:HOH:O	2.13	0.48
1:F:137:GLN:NE2	1:F:143:TRP:HE1	2.10	0.47
1:E:199:ILE:O	1:E:201:PRO:HD3	2.14	0.47
1:B:179:ILE:HG22	1:B:242:ILE:HG12	1.95	0.47
1:C:53:ARG:HE	1:C:55:GLN:HE21	1.62	0.47
1:A:297:ARG:HB3	1:A:298:PRO:HA	1.95	0.47
1:F:182:LEU:HD11	1:F:243:ALA:HA	1.96	0.47
1:E:13:LEU:HD12	1:E:85:SER:HB2	1.96	0.47
1:C:280:LYS:HA	4:C:619:HOH:O	2.14	0.47
1:E:53:ARG:HH11	1:E:53:ARG:HG3	1.79	0.47
1:F:13:LEU:HD12	1:F:85:SER:HB2	1.97	0.47
1:C:252:LEU:HB2	1:C:329:LEU:HD21	1.94	0.47
1:D:138:ARG:HH21	1:D:146:PHE:HD2	1.61	0.47
1:A:121:LEU:HD23	1:A:216:ARG:HD3	1.97	0.47
1:C:308:ASP:HA	4:C:625:HOH:O	2.15	0.47
1:E:128:PRO:O	1:E:131:ILE:HG12	2.15	0.47
1:F:108:SER:HB3	1:F:149:THR:HG22	1.97	0.47
1:C:53:ARG:HE	1:C:55:GLN:NE2	2.12	0.46
1:D:128:PRO:O	1:D:131:ILE:HG12	2.15	0.46
1:A:116:ASP:HB2	1:A:119:VAL:HG23	1.97	0.46
1:A:121:LEU:CD2	1:A:216:ARG:HD3	2.45	0.46
1:F:89:GLN:HG2	1:F:111:PRO:HG2	1.98	0.46
1:B:137:GLN:NE2	1:B:147:ILE:H	2.08	0.46
1:B:153:CYS:HG	3:B:402:COA:HS1	1.44	0.46
1:B:173:GLY:H	1:B:255:SER:HB3	1.81	0.46
1:F:121:LEU:HD23	1:F:216:ARG:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:HIS:CE1	1:A:337:VAL:HG23	2.51	0.46
1:C:333:ILE:HD11	1:C:338:ARG:HG3	1.97	0.46
1:D:28:SER:HB3	4:D:628:HOH:O	2.15	0.46
1:B:252:LEU:HD12	1:B:252:LEU:N	2.31	0.46
1:A:116:ASP:HB2	1:A:119:VAL:CG2	2.46	0.46
1:A:275:GLU:N	1:A:276:PRO:CD	2.79	0.45
1:F:77:MET:O	1:F:80:VAL:N	2.47	0.45
1:E:333:ILE:HD11	1:E:338:ARG:HG3	1.98	0.45
1:A:101:LYS:HE3	1:A:101:LYS:HB2	1.69	0.45
1:D:297:ARG:HB3	1:D:298:PRO:HA	1.98	0.45
1:F:75:LYS:H	1:F:75:LYS:HG2	1.55	0.45
1:A:229:LYS:H	1:A:229:LYS:HD3	1.81	0.45
1:D:53:ARG:HG3	1:D:53:ARG:HH11	1.82	0.45
1:D:89:GLN:HE21	1:D:89:GLN:HB3	1.44	0.45
1:D:9:LYS:HG3	1:D:36:ALA:CB	2.45	0.45
1:E:329:LEU:HD23	1:E:329:LEU:C	2.37	0.45
1:B:34:LYS:HA	1:B:34:LYS:HE2	1.98	0.45
1:D:154:THR:HG21	1:D:180:GLN:NE2	2.32	0.45
1:F:211:ILE:HA	1:F:211:ILE:HD12	1.70	0.45
1:D:121:LEU:HD23	1:D:216:ARG:HG2	1.99	0.45
1:E:213:GLU:O	1:E:217:ILE:HG13	2.17	0.45
1:C:137:GLN:HE22	1:C:147:ILE:H	1.63	0.45
1:F:199:ILE:O	1:F:201:PRO:HD3	2.16	0.44
1:C:297:ARG:HB3	1:C:298:PRO:HA	1.99	0.44
1:B:333:ILE:HD11	1:B:338:ARG:HG3	1.98	0.44
1:A:152:LEU:O	1:A:153:CYS:C	2.56	0.44
1:B:170:LYS:HA	1:B:227:GLU:O	2.17	0.44
1:F:73:ASP:HA	1:F:74:PRO:HD2	1.83	0.44
1:E:89:GLN:HB3	1:E:89:GLN:HE21	1.40	0.44
1:F:276:PRO:HB3	1:F:281:LEU:HD12	2.00	0.44
1:A:13:LEU:HA	1:A:39:ALA:HB3	2.00	0.44
1:D:252:LEU:HB2	1:D:329:LEU:HD21	1.97	0.44
1:C:283:THR:O	1:C:283:THR:HG22	2.18	0.44
1:C:267:GLU:HA	4:C:650:HOH:O	2.14	0.44
1:C:192:SER:O	1:C:196:VAL:HG23	2.18	0.44
1:A:74:PRO:CB	1:A:102:GLU:HG3	2.47	0.43
1:D:355:GLY:HA2	4:D:637:HOH:O	2.17	0.43
1:A:181:SER:HA	1:A:244:THR:OG1	2.17	0.43
1:A:209:LYS:NZ	4:A:727:HOH:O	2.51	0.43
1:D:207:ASP:OD2	4:D:632:HOH:O	2.21	0.43
1:A:57:VAL:HG22	1:A:58:GLY:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ARG:HH21	1:E:146:PHE:HD2	1.65	0.43
1:D:180:GLN:HB3	1:D:248:HIS:CE1	2.53	0.43
1:F:23:TYR:CZ	1:F:341:ALA:HA	2.54	0.43
1:E:275:GLU:N	1:E:276:PRO:CD	2.81	0.43
1:A:261:ALA:HA	1:A:321:GLN:HE22	1.84	0.43
1:C:322:VAL:HA	4:C:604:HOH:O	2.18	0.43
1:C:263:GLU:N	4:C:632:HOH:O	2.51	0.43
1:A:316:VAL:HA	1:A:331:SER:HA	2.01	0.43
1:A:128:PRO:HG3	4:A:708:HOH:O	2.18	0.43
1:E:13:LEU:HA	1:E:39:ALA:HB3	2.01	0.43
1:E:266:LYS:NZ	1:E:293:ASN:ND2	2.67	0.43
1:E:329:LEU:HD23	1:E:329:LEU:O	2.18	0.43
1:F:137:GLN:HE22	1:F:147:ILE:H	1.65	0.42
1:F:126:LEU:HD11	1:F:160:ILE:HA	2.01	0.42
1:A:62:LYS:H	1:A:62:LYS:HG2	1.58	0.42
1:F:297:ARG:HB3	1:F:298:PRO:HA	1.99	0.42
1:B:74:PRO:HG2	1:B:98:GLN:HG3	2.01	0.42
1:A:229:LYS:HE3	4:A:704:HOH:O	2.18	0.42
1:E:95:VAL:HG23	4:E:641:HOH:O	2.18	0.42
1:B:89:GLN:HG2	1:B:111:PRO:HG3	2.01	0.42
1:B:270:GLU:HG3	1:B:291:VAL:HG21	2.02	0.42
3:A:402:COA:H22	4:A:630:HOH:O	2.19	0.42
1:D:19:VAL:HG23	3:D:402:COA:H132	2.02	0.42
1:E:87:LEU:HA	1:E:87:LEU:HD12	1.79	0.42
1:F:165:ILE:HG12	1:F:265:VAL:HG13	2.02	0.42
1:C:158:ALA:O	1:C:161:PRO:HD2	2.20	0.42
1:F:356:TYR:CE2	4:F:629:HOH:O	2.56	0.42
1:B:283:THR:HG22	1:B:283:THR:O	2.20	0.42
1:D:127:ASN:HB2	1:D:130:THR:CG2	2.50	0.41
1:C:199:ILE:O	1:C:201:PRO:HD3	2.20	0.41
1:E:211:ILE:HA	1:E:211:ILE:HD12	1.80	0.41
1:B:211:ILE:HG13	1:B:235:LEU:HB3	2.01	0.41
1:C:328:ARG:HD2	1:C:329:LEU:N	2.36	0.41
1:F:283:THR:O	1:F:283:THR:HG22	2.20	0.41
1:C:77:MET:O	1:C:79:ASP:N	2.53	0.41
1:D:316:VAL:HA	1:D:330:VAL:O	2.20	0.41
3:D:402:COA:H122	4:D:635:HOH:O	2.20	0.41
1:F:136:GLU:O	1:F:140:ARG:HB2	2.21	0.41
1:B:180:GLN:NE2	1:B:239:THR:HB	2.35	0.41
1:F:213:GLU:O	1:F:217:ILE:HG13	2.21	0.41
1:E:137:GLN:NE2	1:E:143:TRP:HE1	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:GLN:HG3	1:C:240:HIS:O	2.21	0.41
1:C:308:ASP:CA	4:C:625:HOH:O	2.68	0.41
1:C:287:LYS:HA	1:C:288:PRO:HD2	1.91	0.41
1:E:73:ASP:HA	1:E:74:PRO:HD2	1.85	0.41
1:B:226:ASP:N	1:B:226:ASP:OD1	2.52	0.41
1:F:178:THR:OG1	1:F:239:THR:HA	2.21	0.41
1:E:23:TYR:CZ	1:E:341:ALA:HA	2.55	0.41
1:E:73:ASP:OD1	1:E:75:LYS:HG2	2.21	0.41
1:D:252:LEU:N	1:D:252:LEU:HD12	2.36	0.41
3:D:402:COA:H22	3:D:402:COA:O5P	2.20	0.41
1:C:119:VAL:HA	1:C:120:PRO:HD3	1.90	0.41
1:A:182:LEU:HG	1:A:244:THR:O	2.21	0.41
1:A:192:SER:HB2	1:B:182:LEU:HD13	2.03	0.41
3:F:402:COA:H22	3:F:402:COA:O5P	2.20	0.41
1:C:96:GLU:OE1	1:C:113:HIS:HD2	2.03	0.41
1:E:136:GLU:O	1:E:140:ARG:HB2	2.21	0.41
1:D:276:PRO:HB3	1:D:281:LEU:HD12	2.01	0.41
1:C:126:LEU:HD11	1:C:160:ILE:HA	2.02	0.41
1:A:53:ARG:HE	1:A:55:GLN:NE2	2.19	0.40
1:E:252:LEU:HB2	1:E:329:LEU:HD21	1.99	0.40
1:E:13:LEU:HD12	1:E:85:SER:CB	2.50	0.40
1:D:182:LEU:HD11	1:D:243:ALA:HA	2.04	0.40
1:C:309:ILE:O	1:C:312:MET:HB2	2.21	0.40
1:E:119:VAL:HA	1:E:120:PRO:HD3	1.93	0.40
1:F:53:ARG:HG3	1:F:53:ARG:HH11	1.86	0.40
1:E:75:LYS:HG2	1:E:75:LYS:H	1.60	0.40
1:E:77:MET:O	1:E:79:ASP:N	2.53	0.40
1:D:136:GLU:O	1:D:140:ARG:HB2	2.21	0.40
1:B:38:LEU:HD13	1:B:48:TYR:CD1	2.56	0.40
1:C:30:HIS:HA	4:C:631:HOH:O	2.21	0.40
1:C:53:ARG:HH21	1:C:55:GLN:HE22	1.70	0.40
1:D:77:MET:C	1:D:79:ASP:H	2.25	0.40
1:E:53:ARG:HE	1:E:55:GLN:HE21	1.67	0.40
1:D:13:LEU:HA	1:D:39:ALA:HB3	2.02	0.40
3:F:402:COA:O1A	3:F:402:COA:O4A	2.39	0.40
1:D:275:GLU:N	1:D:276:PRO:CD	2.84	0.40
1:C:165:ILE:HG12	1:C:265:VAL:HG13	2.04	0.40
1:B:121:LEU:HD11	1:B:151:PRO:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:LYS:NZ	1:F:353:GLU:OE2[3_555]	2.01	0.19

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	352/359 (98%)	333 (95%)	15 (4%)	4 (1%)	17	18
1	B	352/359 (98%)	332 (94%)	17 (5%)	3 (1%)	21	24
1	C	352/359 (98%)	334 (95%)	14 (4%)	4 (1%)	17	18
1	D	352/359 (98%)	334 (95%)	15 (4%)	3 (1%)	21	24
1	E	351/359 (98%)	334 (95%)	14 (4%)	3 (1%)	21	24
1	F	351/359 (98%)	335 (95%)	12 (3%)	4 (1%)	17	18
All	All	2110/2154 (98%)	2002 (95%)	87 (4%)	21 (1%)	19	21

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	76	LEU
1	A	86	PRO
1	D	76	LEU
1	F	76	LEU
1	A	231	GLU
1	C	76	LEU
1	C	86	PRO
1	D	86	PRO
1	D	337	VAL
1	F	337	VAL
1	A	340	ALA
1	B	75	LYS
1	B	170	LYS
1	C	337	VAL
1	F	86	PRO

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Mol	Chain	Res	Type
1	B	86	PRO
1	F	78	ASP
1	E	337	VAL
1	A	337	VAL
1	C	211	ILE
1	E	86	PRO

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	297/302 (98%)	276 (93%)	21 (7%)	18	23
1	B	297/302 (98%)	276 (93%)	21 (7%)	18	23
1	C	297/302 (98%)	262 (88%)	35 (12%)	6	7
1	D	297/302 (98%)	261 (88%)	36 (12%)	6	6
1	E	296/302 (98%)	261 (88%)	35 (12%)	6	7
1	F	296/302 (98%)	261 (88%)	35 (12%)	6	7
All	All	1780/1812 (98%)	1597 (90%)	183 (10%)	9	10

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	29	ASN
1	A	34	LYS
1	A	51	VAL
1	A	55	GLN
1	A	62	LYS
1	A	64	ILE
1	A	74	PRO
1	A	75	LYS
1	A	78	ASP
1	A	87	LEU
1	A	131	ILE

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Mol	Chain	Res	Type
1	A	140	ARG
1	A	143	TRP
1	A	144	LYS
1	A	153	CYS
1	A	209	LYS
1	A	222	LYS
1	A	229	LYS
1	A	263	GLU
1	A	280	LYS
1	B	6	ARG
1	B	7	THR
1	B	50	GLU
1	B	55	GLN
1	B	62	LYS
1	B	68	GLU
1	B	78	ASP
1	B	79	ASP
1	B	87	LEU
1	B	98	GLN
1	B	112	ASP
1	B	140	ARG
1	B	143	TRP
1	B	211	ILE
1	B	255	SER
1	B	257	LYS
1	B	320	LYS
1	B	325	ARG
1	B	329	LEU
1	B	353	GLU
1	B	359	LYS
1	C	7	THR
1	C	9	LYS
1	C	34	LYS
1	C	41	LYS
1	C	43	SER
1	C	55	GLN
1	C	62	LYS
1	C	64	ILE
1	C	75	LYS
1	C	76	LEU
1	C	79	ASP
1	C	87	LEU

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Mol	Chain	Res	Type
1	C	89	GLN
1	C	98	GLN
1	C	132	SER
1	C	136	GLU
1	C	139	LYS
1	C	143	TRP
1	C	144	LYS
1	C	209	LYS
1	C	211	ILE
1	C	229	LYS
1	C	230	LEU
1	C	231	GLU
1	C	257	LYS
1	C	259	GLU
1	C	263	GLU
1	C	273	ARG
1	C	287	LYS
1	C	319	LEU
1	C	320	LYS
1	C	329	LEU
1	C	353	GLU
1	C	358	GLU
1	C	359	LYS
1	D	6	ARG
1	D	7	THR
1	D	9	LYS
1	D	34	LYS
1	D	41	LYS
1	D	43	SER
1	D	55	GLN
1	D	62	LYS
1	D	64	ILE
1	D	75	LYS
1	D	76	LEU
1	D	79	ASP
1	D	87	LEU
1	D	89	GLN
1	D	98	GLN
1	D	132	SER
1	D	136	GLU
1	D	139	LYS
1	D	143	TRP

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Mol	Chain	Res	Type
1	D	144	LYS
1	D	209	LYS
1	D	211	ILE
1	D	219	SER
1	D	228	PRO
1	D	229	LYS
1	D	231	GLU
1	D	257	LYS
1	D	263	GLU
1	D	273	ARG
1	D	287	LYS
1	D	319	LEU
1	D	320	LYS
1	D	329	LEU
1	D	353	GLU
1	D	358	GLU
1	D	359	LYS
1	E	7	THR
1	E	9	LYS
1	E	34	LYS
1	E	41	LYS
1	E	43	SER
1	E	55	GLN
1	E	62	LYS
1	E	64	ILE
1	E	75	LYS
1	E	76	LEU
1	E	78	ASP
1	E	79	ASP
1	E	87	LEU
1	E	89	GLN
1	E	98	GLN
1	E	132	SER
1	E	136	GLU
1	E	139	LYS
1	E	143	TRP
1	E	144	LYS
1	E	153	CYS
1	E	209	LYS
1	E	211	ILE
1	E	228	PRO
1	E	229	LYS

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Mol	Chain	Res	Type
1	E	231	GLU
1	E	257	LYS
1	E	263	GLU
1	E	273	ARG
1	E	287	LYS
1	E	319	LEU
1	E	320	LYS
1	E	329	LEU
1	E	353	GLU
1	E	359	LYS
1	F	7	THR
1	F	9	LYS
1	F	34	LYS
1	F	41	LYS
1	F	43	SER
1	F	55	GLN
1	F	62	LYS
1	F	64	ILE
1	F	75	LYS
1	F	76	LEU
1	F	79	ASP
1	F	87	LEU
1	F	89	GLN
1	F	98	GLN
1	F	136	GLU
1	F	139	LYS
1	F	143	TRP
1	F	144	LYS
1	F	209	LYS
1	F	211	ILE
1	F	229	LYS
1	F	230	LEU
1	F	231	GLU
1	F	257	LYS
1	F	259	GLU
1	F	263	GLU
1	F	273	ARG
1	F	280	LYS
1	F	287	LYS
1	F	319	LEU
1	F	320	LYS
1	F	329	LEU

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Mol	Chain	Res	Type
1	F	353	GLU
1	F	358	GLU
1	F	359	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	137	GLN
1	A	180	GLN
1	A	293	ASN
1	A	321	GLN
1	B	55	GLN
1	B	59	GLN
1	B	129	HIS
1	B	137	GLN
1	B	180	GLN
1	B	293	ASN
1	B	321	GLN
1	C	55	GLN
1	C	89	GLN
1	C	129	HIS
1	C	137	GLN
1	C	180	GLN
1	C	293	ASN
1	C	321	GLN
1	D	55	GLN
1	D	89	GLN
1	D	129	HIS
1	D	137	GLN
1	D	180	GLN
1	D	293	ASN
1	D	321	GLN
1	E	55	GLN
1	E	89	GLN
1	E	129	HIS
1	E	137	GLN
1	E	180	GLN
1	E	246	HIS
1	E	293	ASN
1	E	321	GLN
1	F	55	GLN

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Mol	Chain	Res	Type
1	F	89	GLN
1	F	129	HIS
1	F	137	GLN
1	F	180	GLN
1	F	246	HIS
1	F	293	ASN
1	F	321	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
3	COA	A	402	2	40,50,50	1.60	10 (25%)	50,75,75	3.91	28 (56%)
3	COA	B	402	2	40,50,50	1.18	3 (7%)	50,75,75	4.05	30 (60%)
3	COA	C	402	2	40,50,50	0.88	1 (2%)	50,75,75	2.68	13 (26%)
3	COA	D	402	2	40,50,50	0.79	0	50,75,75	2.19	10 (20%)
3	COA	E	402	2	40,50,50	0.87	1 (2%)	50,75,75	2.46	14 (28%)
3	COA	F	402	2	40,50,50	0.83	1 (2%)	50,75,75	2.36	10 (20%)

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
3	COA	A	402	2	-	0/44/64/64	0/3/3/3
3	COA	B	402	2	-	0/44/64/64	0/3/3/3
3	COA	C	402	2	-	0/44/64/64	0/3/3/3
3	COA	D	402	2	-	0/44/64/64	0/3/3/3
3	COA	E	402	2	-	0/44/64/64	0/3/3/3
3	COA	F	402	2	-	0/44/64/64	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	COA	O4B-C1B	-3.33	1.37	1.41
3	A	402	COA	C4A-N3A	-3.25	1.30	1.35
3	A	402	COA	C5A-N7A	-2.56	1.30	1.39
3	A	402	COA	P3B-O9A	-2.19	1.46	1.54
3	A	402	COA	O6A-CCP	-2.09	1.36	1.43
3	B	402	COA	C2A-N1A	-2.05	1.30	1.33
3	A	402	COA	O5P-C5P	2.04	1.27	1.23
3	C	402	COA	OAP-CAP	2.12	1.46	1.42
3	E	402	COA	O4B-C1B	2.29	1.44	1.41
3	B	402	COA	C5P-N4P	2.42	1.39	1.33
3	A	402	COA	OAP-CAP	2.51	1.47	1.42
3	A	402	COA	C7P-C6P	2.53	1.59	1.51
3	A	402	COA	C2A-N3A	2.57	1.36	1.32
3	B	402	COA	CEP-CBP	2.66	1.59	1.53
3	F	402	COA	O4B-C1B	3.03	1.45	1.41
3	A	402	COA	C9P-N8P	3.53	1.41	1.33

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	COA	N3A-C2A-N1A	-11.88	119.80	128.89
3	D	402	COA	N3A-C2A-N1A	-10.09	121.17	128.89
3	F	402	COA	N3A-C2A-N1A	-10.08	121.18	128.89
3	B	402	COA	N3A-C2A-N1A	-9.41	121.69	128.89
3	C	402	COA	CDP-CBP-CCP	-9.27	96.48	108.50
3	E	402	COA	N3A-C2A-N1A	-9.02	121.99	128.89
3	C	402	COA	N3A-C2A-N1A	-8.59	122.32	128.89
3	B	402	COA	O5P-C5P-C6P	-7.33	109.33	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	COA	C6P-C7P-N8P	-7.23	96.02	111.88
3	F	402	COA	C6P-C7P-N8P	-6.69	97.20	111.88
3	A	402	COA	O6A-CCP-CBP	-6.65	99.86	110.55
3	E	402	COA	C6P-C7P-N8P	-6.60	97.41	111.88
3	B	402	COA	CEP-CBP-CDP	-6.49	96.25	109.28
3	C	402	COA	C6P-C7P-N8P	-6.46	97.71	111.88
3	A	402	COA	C2P-C3P-N4P	-5.93	100.65	112.37
3	A	402	COA	CEP-CBP-CDP	-5.87	97.50	109.28
3	D	402	COA	C6P-C7P-N8P	-5.72	99.32	111.88
3	E	402	COA	CDP-CBP-CCP	-5.51	101.36	108.50
3	B	402	COA	C2B-C1B-N9A	-5.17	106.39	114.29
3	B	402	COA	C4B-O4B-C1B	-5.11	104.11	109.72
3	E	402	COA	C2P-C3P-N4P	-5.06	102.39	112.37
3	D	402	COA	C2P-C3P-N4P	-4.91	102.67	112.37
3	F	402	COA	C2P-C3P-N4P	-4.44	103.60	112.37
3	F	402	COA	P2A-O3A-P1A	-4.34	120.56	132.73
3	A	402	COA	P2A-O3A-P1A	-4.20	120.93	132.73
3	C	402	COA	C2P-C3P-N4P	-4.16	104.16	112.37
3	B	402	COA	O6A-CCP-CBP	-4.16	103.86	110.55
3	E	402	COA	P2A-O3A-P1A	-4.04	121.38	132.73
3	B	402	COA	O6A-P2A-O4A	-3.81	94.82	109.62
3	E	402	COA	O5P-C5P-C6P	-3.77	115.47	121.98
3	A	402	COA	C6P-C7P-N8P	-3.68	103.80	111.88
3	A	402	COA	O5B-C5B-C4B	-3.48	96.30	109.12
3	B	402	COA	P2A-O3A-P1A	-3.46	123.01	132.73
3	C	402	COA	C4B-O4B-C1B	-3.35	106.04	109.72
3	A	402	COA	C4A-C5A-N7A	-3.29	106.45	109.48
3	A	402	COA	O5B-P1A-O1A	-3.26	96.97	109.62
3	F	402	COA	CDP-CBP-CCP	-3.19	104.36	108.50
3	A	402	COA	C2B-C1B-N9A	-3.14	109.50	114.29
3	E	402	COA	C4B-O4B-C1B	-3.08	106.33	109.72
3	C	402	COA	P2A-O3A-P1A	-2.78	124.93	132.73
3	D	402	COA	P2A-O3A-P1A	-2.75	125.00	132.73
3	D	402	COA	O5P-C5P-C6P	-2.69	117.34	121.98
3	C	402	COA	C4A-C5A-N7A	-2.68	107.01	109.48
3	B	402	COA	C5B-C4B-C3B	-2.58	105.02	114.31
3	B	402	COA	O3A-P1A-O5B	-2.55	96.17	102.94
3	C	402	COA	C1B-N9A-C4A	-2.50	123.16	126.94
3	B	402	COA	O9A-P3B-O7A	-2.49	102.57	110.58
3	E	402	COA	O3A-P1A-O5B	-2.44	96.45	102.94
3	A	402	COA	C1B-N9A-C4A	-2.41	123.30	126.94
3	B	402	COA	C2B-C3B-C4B	-2.40	98.78	103.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	COA	C4B-O4B-C1B	-2.39	107.09	109.72
3	A	402	COA	O5A-P2A-O6A	-2.37	96.52	108.46
3	E	402	COA	C2B-C1B-N9A	-2.36	110.68	114.29
3	F	402	COA	C1B-N9A-C4A	-2.28	123.50	126.94
3	A	402	COA	O4B-C4B-C5B	-2.15	101.61	109.32
3	B	402	COA	O3B-C3B-C2B	-2.06	103.49	111.51
3	F	402	COA	O5P-C5P-C6P	-2.04	118.47	121.98
3	A	402	COA	C3P-N4P-C5P	2.02	126.76	122.79
3	D	402	COA	C7P-N8P-C9P	2.03	126.54	122.53
3	C	402	COA	CDP-CBP-CAP	2.03	113.05	109.34
3	A	402	COA	C5B-C4B-C3B	2.06	121.75	114.31
3	B	402	COA	O2A-P1A-O5B	2.17	119.42	108.46
3	E	402	COA	C6P-C5P-N4P	2.29	120.44	116.46
3	A	402	COA	O3B-P3B-O7A	2.35	112.98	107.11
3	B	402	COA	O5B-C5B-C4B	2.37	117.84	109.12
3	C	402	COA	CEP-CBP-CDP	2.37	114.04	109.28
3	A	402	COA	O5A-P2A-O3A	2.47	116.31	105.09
3	F	402	COA	O6A-CCP-CBP	2.57	114.68	110.55
3	D	402	COA	O8A-P3B-O7A	2.59	118.91	110.58
3	B	402	COA	C7P-N8P-C9P	2.62	127.71	122.53
3	F	402	COA	CEP-CBP-CCP	2.68	111.98	108.50
3	D	402	COA	O6A-CCP-CBP	2.69	114.88	110.55
3	E	402	COA	O4B-C1B-N9A	2.70	113.75	108.10
3	D	402	COA	O4B-C1B-N9A	2.74	113.84	108.10
3	C	402	COA	C7P-C6P-C5P	2.78	116.90	112.31
3	A	402	COA	O3A-P1A-O5B	2.83	110.45	102.94
3	E	402	COA	CDP-CBP-CAP	2.94	114.71	109.34
3	A	402	COA	O2A-P1A-O3A	2.97	118.59	105.09
3	B	402	COA	O4B-C1B-N9A	3.03	114.45	108.10
3	E	402	COA	CEP-CBP-CCP	3.05	112.45	108.50
3	A	402	COA	CDP-CBP-CAP	3.26	115.29	109.34
3	E	402	COA	C7P-N8P-C9P	3.33	129.13	122.53
3	A	402	COA	O9P-C9P-N8P	3.40	129.91	123.08
3	F	402	COA	O4B-C1B-N9A	3.58	115.58	108.10
3	B	402	COA	O4B-C4B-C3B	3.67	113.31	104.86
3	B	402	COA	O2A-P1A-O3A	3.73	122.03	105.09
3	B	402	COA	C3P-N4P-C5P	3.76	130.19	122.79
3	C	402	COA	C7P-N8P-C9P	4.19	130.82	122.53
3	A	402	COA	CEP-CBP-CAP	4.54	117.62	109.34
3	B	402	COA	C7P-C6P-C5P	4.62	119.93	112.31
3	B	402	COA	O5A-P2A-O3A	4.88	127.22	105.09
3	A	402	COA	O4B-C1B-N9A	4.93	118.43	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	COA	O9A-P3B-O8A	4.96	126.25	107.38
3	B	402	COA	P3B-O3B-C3B	5.13	133.86	121.56
3	B	402	COA	C6P-C5P-N4P	5.47	125.95	116.46
3	B	402	COA	CEP-CBP-CAP	5.86	120.05	109.34
3	A	402	COA	O9A-P3B-O8A	6.04	130.39	107.38
3	A	402	COA	P3B-O3B-C3B	6.36	136.82	121.56
3	C	402	COA	CEP-CBP-CCP	6.37	116.76	108.50
3	B	402	COA	CDP-CBP-CAP	7.49	123.03	109.34
3	A	402	COA	C7P-N8P-C9P	7.76	137.89	122.53
3	A	402	COA	CEP-CBP-CCP	8.19	119.12	108.50
3	B	402	COA	CDP-CBP-CCP	8.24	119.18	108.50
3	B	402	COA	CEP-CBP-CCP	8.93	120.08	108.50
3	A	402	COA	CDP-CBP-CCP	9.15	120.36	108.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	COA	1	0
3	B	402	COA	3	0
3	C	402	COA	1	0
3	D	402	COA	4	0
3	E	402	COA	1	0
3	F	402	COA	2	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	354/359 (98%)	-0.07	7 (1%) 68 75	11, 29, 59, 105	0
1	B	354/359 (98%)	-0.03	5 (1%) 78 83	14, 34, 63, 94	0
1	C	354/359 (98%)	0.96	64 (18%) 2 3	53, 87, 132, 173	0
1	D	354/359 (98%)	2.02	137 (38%) 0 0	64, 116, 187, 220	0
1	E	353/359 (98%)	1.20	81 (22%) 1 1	53, 98, 162, 193	0
1	F	353/359 (98%)	1.36	101 (28%) 1 1	61, 114, 181, 216	0
All	All	2122/2154 (98%)	0.91	395 (18%) 2 2	11, 84, 164, 220	0

All (395) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	84	PHE	11.1
1	D	94	PRO	9.6
1	D	65	ALA	9.1
1	D	344	GLY	8.9
1	D	67	MET	8.8
1	D	107	ILE	8.7
1	D	6	ARG	8.4
1	D	78	ASP	8.1
1	E	230	LEU	8.0
1	D	343	GLY	7.6
1	D	23	TYR	7.6
1	F	229	LYS	7.5
1	D	359	LYS	7.3
1	D	345	ILE	7.2
1	D	64	ILE	7.1
1	F	145	GLY	7.0
1	D	31	PRO	6.8
1	D	44	VAL	6.8
1	D	341	ALA	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	139	LYS	6.5
1	C	140	ARG	6.4
1	E	261	ALA	6.3
1	D	72	THR	6.0
1	D	109	ASN	6.0
1	D	8	LEU	6.0
1	C	225	VAL	5.8
1	D	148	VAL	5.8
1	D	83	ILE	5.8
1	D	85	SER	5.5
1	D	86	PRO	5.5
1	E	308	ASP	5.5
1	F	40	GLY	5.4
1	D	145	GLY	5.3
1	C	276	PRO	5.3
1	F	140	ARG	5.2
1	D	140	ARG	5.1
1	F	188	PRO	5.1
1	F	64	ILE	5.1
1	F	139	LYS	5.0
1	D	42	GLY	5.0
1	E	271	ASN	4.9
1	C	359	LYS	4.9
1	D	40	GLY	4.9
1	F	68	GLU	4.8
1	D	11	ALA	4.8
1	C	144	LYS	4.8
1	E	262	ALA	4.7
1	D	307	GLY	4.7
1	D	353	GLU	4.7
1	C	139	LYS	4.7
1	D	13	LEU	4.7
1	D	340	ALA	4.6
1	F	46	LYS	4.6
1	F	103	GLY	4.6
1	C	142	GLU	4.5
1	F	109	ASN	4.5
1	E	171	MET	4.5
1	D	98	GLN	4.5
1	D	19	VAL	4.5
1	F	84	PHE	4.4
1	E	139	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	14	GLY	4.4
1	D	91	ALA	4.4
1	E	339	GLY	4.4
1	D	81	ASP	4.4
1	E	155	ALA	4.4
1	E	170	LYS	4.4
1	F	129	HIS	4.4
1	F	19	VAL	4.3
1	D	108	SER	4.3
1	D	219	SER	4.3
1	D	73	ASP	4.3
1	D	12	ILE	4.3
1	F	75	LYS	4.3
1	D	280	LYS	4.2
1	E	258	GLU	4.2
1	D	225	VAL	4.2
1	C	286	SER	4.2
1	D	61	PRO	4.2
1	F	91	ALA	4.2
1	D	69	ILE	4.2
1	F	226	ASP	4.1
1	E	340	ALA	4.1
1	D	50	GLU	4.1
1	E	325	ARG	4.1
1	C	267	GLU	4.1
1	E	260	THR	4.1
1	F	141	ARG	4.1
1	E	117	PRO	4.1
1	D	29	ASN	4.1
1	D	336	THR	4.1
1	D	45	GLY	4.0
1	D	71	PRO	4.0
1	D	218	LEU	4.0
1	C	135	ASP	4.0
1	F	143	TRP	4.0
1	E	290	ILE	4.0
1	D	337	VAL	3.9
1	E	251	VAL	3.9
1	E	224	ASN	3.9
1	E	338	ARG	3.9
1	F	95	VAL	3.9
1	C	145	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	173	GLY	3.9
1	F	37	TYR	3.9
1	F	132	SER	3.8
1	F	144	LYS	3.8
1	D	75	LYS	3.8
1	F	227	GLU	3.8
1	E	169	TYR	3.8
1	C	101	LYS	3.8
1	E	29	ASN	3.7
1	D	63	GLU	3.7
1	E	150	THR	3.7
1	F	66	ASP	3.7
1	F	359	LYS	3.7
1	D	93	GLY	3.7
1	D	274	GLY	3.7
1	E	284	ALA	3.7
1	C	62	LYS	3.6
1	E	140	ARG	3.6
1	D	208	ALA	3.6
1	D	215	PHE	3.6
1	E	232	ASP	3.6
1	C	249	TYR	3.6
1	D	46	LYS	3.6
1	F	63	GLU	3.6
1	E	64	ILE	3.6
1	D	10	ALA	3.6
1	F	307	GLY	3.5
1	D	338	ARG	3.5
1	F	214	ILE	3.5
1	C	6	ARG	3.5
1	F	61	PRO	3.5
1	F	344	GLY	3.5
1	D	176	ILE	3.5
1	D	135	ASP	3.5
1	D	251	VAL	3.5
1	D	82	ILE	3.5
1	E	225	VAL	3.4
1	C	261	ALA	3.4
1	F	65	ALA	3.4
1	F	208	ALA	3.4
1	E	156	GLN	3.4
1	D	276	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	117	PRO	3.4
1	E	321	GLN	3.4
1	C	75	LYS	3.4
1	D	60	VAL	3.4
1	F	112	ASP	3.4
1	C	281	LEU	3.4
1	F	73	ASP	3.4
1	E	107	ILE	3.4
1	C	143	TRP	3.3
1	C	340	ALA	3.3
1	D	129	HIS	3.3
1	F	86	PRO	3.3
1	E	324	LYS	3.3
1	F	42	GLY	3.3
1	A	6	ARG	3.3
1	D	339	GLY	3.3
1	D	252	LEU	3.3
1	D	351	LEU	3.3
1	D	47	PRO	3.3
1	D	35	PRO	3.2
1	D	49	GLY	3.2
1	E	129	HIS	3.2
1	D	150	THR	3.2
1	E	248	HIS	3.2
1	F	101	LYS	3.2
1	F	232	ASP	3.2
1	F	187	TYR	3.2
1	F	52	VAL	3.2
1	E	249	TYR	3.2
1	D	20	GLY	3.2
1	D	43	SER	3.2
1	E	286	SER	3.2
1	F	118	ASP	3.2
1	D	281	LEU	3.2
1	F	151	PRO	3.2
1	D	358	GLU	3.2
1	F	115	PHE	3.2
1	D	48	TYR	3.2
1	D	62	LYS	3.1
1	C	19	VAL	3.1
1	D	133	LEU	3.1
1	F	9	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	308	ASP	3.1
1	F	258	GLU	3.1
1	D	333	ILE	3.1
1	D	203	GLY	3.1
1	F	156	GLN	3.1
1	D	100	ALA	3.0
1	C	252	LEU	3.0
1	C	271	ASN	3.0
1	C	308	ASP	3.0
1	D	342	GLY	3.0
1	F	142	GLU	3.0
1	E	106	VAL	3.0
1	D	112	ASP	3.0
1	D	122	LEU	3.0
1	D	106	VAL	3.0
1	D	212	LYS	3.0
1	C	141	ARG	3.0
1	D	175	PHE	3.0
1	C	358	GLU	3.0
1	C	159	ALA	2.9
1	C	262	ALA	2.9
1	D	146	PHE	2.9
1	E	179	ILE	2.9
1	D	177	THR	2.9
1	F	31	PRO	2.9
1	D	136	GLU	2.9
1	E	135	ASP	2.9
1	E	31	PRO	2.8
1	C	84	PHE	2.8
1	C	269	LEU	2.8
1	D	15	ALA	2.8
1	D	348	ALA	2.8
1	F	233	VAL	2.8
1	E	109	ASN	2.8
1	D	38	LEU	2.8
1	E	252	LEU	2.8
1	F	43	SER	2.8
1	C	278	ASP	2.8
1	E	178	THR	2.8
1	F	49	GLY	2.8
1	D	52	VAL	2.8
1	E	264	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	177	THR	2.8
1	C	44	VAL	2.7
1	D	334	HIS	2.7
1	D	144	LYS	2.7
1	E	159	ALA	2.7
1	E	341	ALA	2.7
1	E	227	GLU	2.7
1	E	233	VAL	2.7
1	F	159	ALA	2.7
1	C	280	LYS	2.7
1	E	259	GLU	2.7
1	D	156	GLN	2.7
1	E	32	TYR	2.7
1	C	251	VAL	2.7
1	D	22	GLU	2.7
1	F	62	LYS	2.7
1	C	118	ASP	2.7
1	C	259	GLU	2.7
1	F	231	GLU	2.7
1	E	268	THR	2.7
1	C	226	ASP	2.7
1	A	19	VAL	2.7
1	D	18	LEU	2.6
1	E	30	HIS	2.6
1	D	7	THR	2.6
1	C	229	LYS	2.6
1	F	41	LYS	2.6
1	D	211	ILE	2.6
1	E	294	GLU	2.6
1	E	310	PRO	2.6
1	F	353	GLU	2.6
1	C	343	GLY	2.6
1	F	257	LYS	2.6
1	E	217	ILE	2.6
1	C	257	LYS	2.6
1	E	62	LYS	2.6
1	D	90	GLY	2.6
1	F	155	ALA	2.6
1	E	358	GLU	2.6
1	D	32	TYR	2.6
1	D	246	HIS	2.5
1	F	203	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	258	GLU	2.5
1	F	150	THR	2.5
1	D	214	ILE	2.5
1	E	295	ASP	2.5
1	F	69	ILE	2.5
1	D	115	PHE	2.5
1	F	228	PRO	2.5
1	C	321	GLN	2.5
1	F	325	ARG	2.5
1	F	225	VAL	2.5
1	F	160	ILE	2.5
1	E	283	THR	2.5
1	F	154	THR	2.5
1	E	123	VAL	2.5
1	F	146	PHE	2.5
1	F	175	PHE	2.5
1	C	7	THR	2.5
1	F	89	GLN	2.5
1	F	92	ALA	2.4
1	E	320	LYS	2.4
1	C	158	ALA	2.4
1	F	136	GLU	2.4
1	F	230	LEU	2.4
1	D	187	TYR	2.4
1	F	80	VAL	2.4
1	D	99	PHE	2.4
1	D	66	ASP	2.4
1	D	278	ASP	2.4
1	F	252	LEU	2.4
1	E	153	CYS	2.4
1	E	277	GLN	2.4
1	C	265	VAL	2.4
1	F	114	ARG	2.4
1	E	307	GLY	2.4
1	D	21	ILE	2.4
1	F	107	ILE	2.4
1	A	84	PHE	2.4
1	B	153	CYS	2.4
1	D	97	GLU	2.3
1	C	123	VAL	2.3
1	F	333	ILE	2.3
1	D	174	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	347	ALA	2.3
1	E	7	THR	2.3
1	F	158	ALA	2.3
1	F	79	ASP	2.3
1	C	171	MET	2.3
1	F	104	PHE	2.3
1	E	118	ASP	2.3
1	E	19	VAL	2.3
1	F	205	GLY	2.3
1	F	354	LYS	2.3
1	A	345	ILE	2.3
1	E	138	ARG	2.3
1	C	344	GLY	2.3
1	C	325	ARG	2.3
1	F	90	GLY	2.2
1	F	339	GLY	2.2
1	C	164	ALA	2.2
1	F	72	THR	2.2
1	C	352	VAL	2.2
1	D	80	VAL	2.2
1	E	314	VAL	2.2
1	F	340	ALA	2.2
1	D	132	SER	2.2
1	C	175	PHE	2.2
1	E	122	LEU	2.2
1	C	316	VAL	2.2
1	F	219	SER	2.2
1	F	251	VAL	2.2
1	D	117	PRO	2.2
1	E	58	GLY	2.2
1	C	294	GLU	2.2
1	D	142	GLU	2.2
1	F	157	GLY	2.2
1	C	264	LYS	2.2
1	A	314	VAL	2.2
1	D	95	VAL	2.2
1	F	337	VAL	2.2
1	D	27	LEU	2.2
1	E	34	LYS	2.2
1	F	29	ASN	2.2
1	E	163	GLY	2.2
1	C	23	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	88	PRO	2.2
1	B	162	LEU	2.2
1	F	204	ASP	2.1
1	D	54	TRP	2.1
1	E	231	GLU	2.1
1	C	293	ASN	2.1
1	D	92	ALA	2.1
1	B	107	ILE	2.1
1	F	173	GLY	2.1
1	F	47	PRO	2.1
1	D	229	LYS	2.1
1	B	252	LEU	2.1
1	D	121	LEU	2.1
1	E	226	ASP	2.1
1	E	333	ILE	2.1
1	F	44	VAL	2.1
1	C	232	ASP	2.1
1	D	141	ARG	2.1
1	C	76	LEU	2.1
1	A	340	ALA	2.1
1	F	280	LYS	2.1
1	E	211	ILE	2.1
1	E	267	GLU	2.1
1	D	232	ASP	2.1
1	F	67	MET	2.1
1	D	173	GLY	2.1
1	D	257	LYS	2.1
1	C	136	GLU	2.1
1	C	254	VAL	2.1
1	D	26	MET	2.1
1	F	358	GLU	2.0
1	D	184	GLY	2.0
1	E	175	PHE	2.0
1	E	282	PRO	2.0
1	B	160	ILE	2.0
1	E	229	LYS	2.0
1	F	94	PRO	2.0
1	D	190	ILE	2.0
1	C	320	LYS	2.0
1	A	252	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(\AA^2)	Q<0.9
3	COA	A	402	48/48	0.95	0.12	-0.42	31,40,58,72	0
3	COA	B	402	48/48	0.96	0.11	-0.46	31,43,61,70	0
3	COA	E	402	48/48	0.94	0.12	-0.65	63,73,97,106	0
3	COA	C	402	48/48	0.95	0.12	-0.83	63,69,100,108	0
3	COA	F	402	48/48	0.92	0.15	-0.96	133,144,156,160	0
3	COA	D	402	48/48	0.88	0.17	-1.07	120,144,169,175	0
2	MG	C	401	1/1	0.94	0.12	-	75,75,75,75	0
2	MG	E	401	1/1	0.92	0.08	-	78,78,78,78	0
2	MG	D	401	1/1	0.62	0.16	-	125,125,125,125	0
2	MG	A	401	1/1	0.56	0.17	-	52,52,52,52	0
2	MG	B	401	1/1	0.92	0.10	-	48,48,48,48	0
2	MG	F	401	1/1	0.89	0.11	-	127,127,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.