



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:42 PM UTC

PDB ID : 1JLL / pdb_00001jll
Title : Crystal Structure Analysis of the E197betaA Mutant of E. coli SCS
Authors : Fraser, M.E.
Deposited on : 2001-07-16
Resolution : 2.69 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

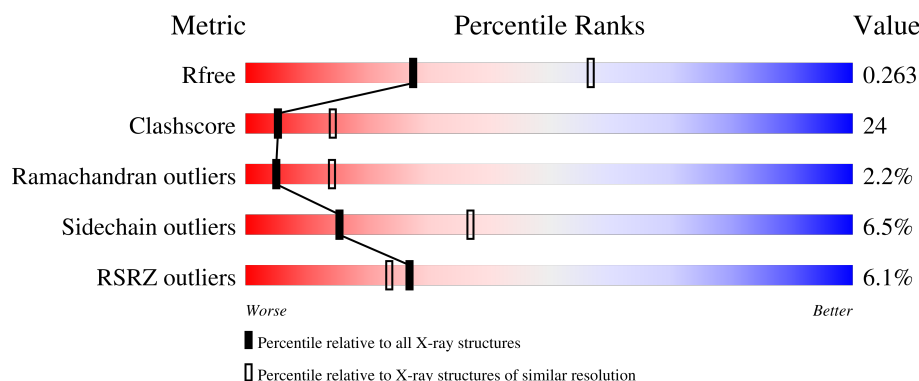
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	3% 55% 39% 6%
1	D	288	6% 51% 42% 7%
2	B	388	11% 56% 35% 9%
2	E	388	3% 56% 36% 6%

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
3	PO4	D	1601	-	-	X	-
4	COA	B	1903	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10255 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 succinyl-CoA synthetase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2069	1313	346	399	11			
1	D	287	Total	C	N	O	S	0	0	0
			2069	1313	346	399	11			

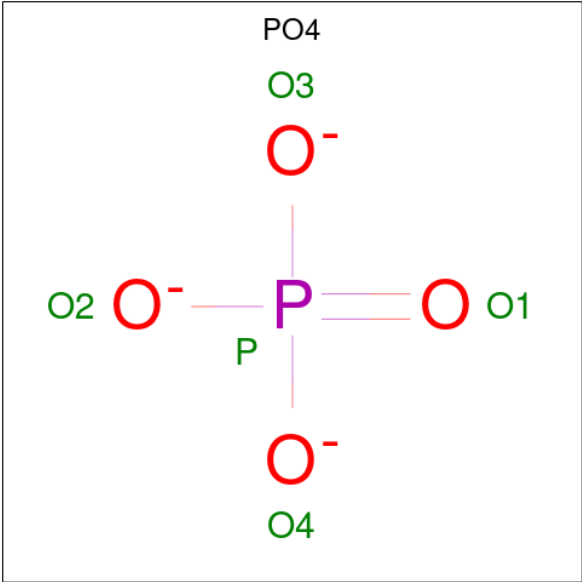
- Molecule 2 is a protein called succinyl-CoA synthetase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	388	Total	C	N	O	S	0	0	0
			2904	1834	509	548	13			
2	E	385	Total	C	N	O	S	0	0	0
			2881	1821	505	542	13			

There are 2 discrepancies between the modelled and reference sequences:

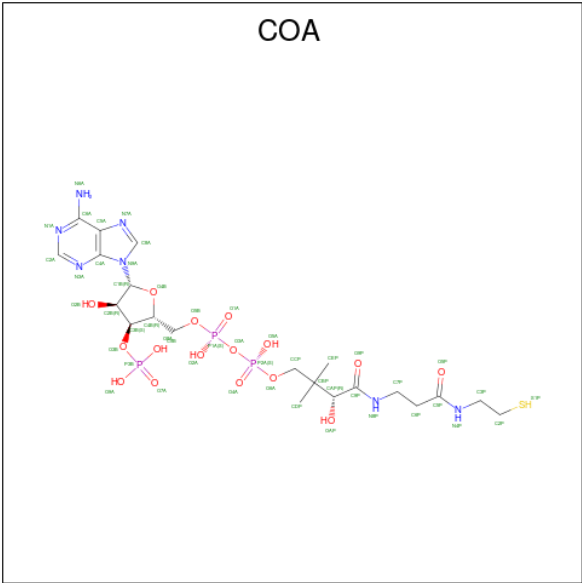
Chain	Residue	Modelled	Actual	Comment	Reference
B	197	ALA	GLU	engineered mutation	UNP P0A836
E	197	ALA	GLU	engineered mutation	UNP P0A836

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	P		0	0
			5	4	1			
3	D	1	Total	O	P		0	0
			5	4	1			

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
4	B	1	Total	C	N	O	S	0	0
			17	11	2	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
4	E	1	Total	C	N	O	S	0	0
			8	5	1	1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	57	Total	O	0	0
			57	57		
6	B	46	Total	O	0	0
			46	46		
6	D	34	Total	O	0	0
			34	34		

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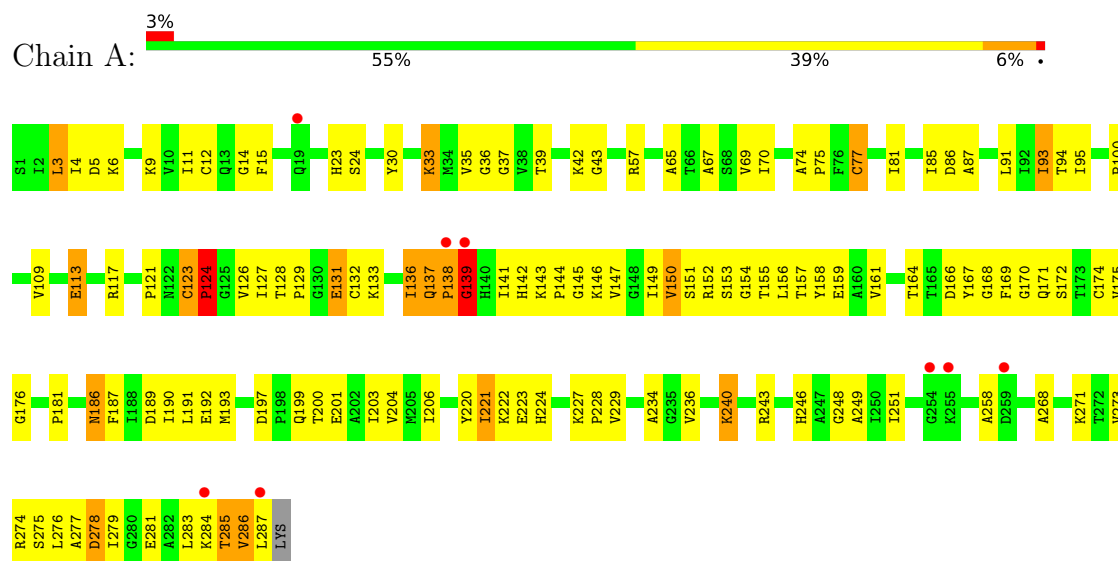
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	56	Total	O	0	0
			56	56		

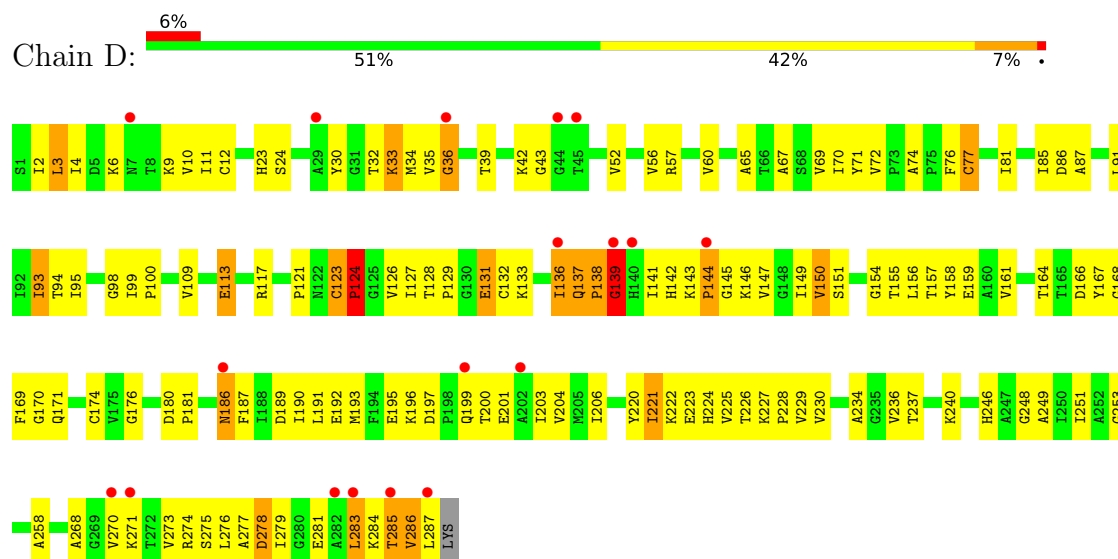
3 Residue-property plots

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

- Molecule 1: succinyl-CoA synthetase alpha subunit



- Molecule 1: succinyl-CoA synthetase alpha subunit



- Molecule 2: succinyl-CoA synthetase beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	97.06Å 97.06Å 389.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.38 – 2.69 34.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.5 (34.38-2.69) 91.5 (34.38-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.259 0.228 , 0.263	Depositor DCC
R_{free} test set	1000 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10255	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, SO4, PO4

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	1.02	2/2103 (0.1%)	1.30	23/2849 (0.8%)
1	D	0.97	3/2103 (0.1%)	1.27	18/2849 (0.6%)
2	B	0.92	2/2946 (0.1%)	1.23	24/3984 (0.6%)
2	E	0.92	2/2923 (0.1%)	1.27	31/3956 (0.8%)
All	All	0.95	9/10075 (0.1%)	1.27	96/13638 (0.7%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	69	VAL	CA-CB	7.83	1.63	1.54
2	E	124	MET	SD-CE	6.88	1.96	1.79
2	E	182	MET	SD-CE	-6.59	1.63	1.79
1	A	136	ILE	CA-CB	6.40	1.61	1.54
1	A	124	PRO	CA-C	5.91	1.60	1.52
2	B	232	MET	SD-CE	-5.50	1.65	1.79
2	B	182	MET	SD-CE	-5.20	1.66	1.79
1	D	74	ALA	CA-CB	-5.18	1.49	1.54
1	D	136	ILE	CA-CB	5.06	1.60	1.54

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	194	ALA	N-CA-C	-9.93	101.67	113.88
2	E	194	ALA	N-CA-C	-9.67	101.98	113.88
2	B	76	TRP	N-CA-C	9.40	123.26	111.69
2	E	76	TRP	N-CA-C	9.22	123.03	111.69
2	E	201	LEU	N-CA-C	-8.32	95.01	108.41
2	B	201	LEU	N-CA-C	-8.21	95.20	108.41
2	E	154	GLY	CA-C-N	-7.73	111.80	119.76
2	E	154	GLY	C-N-CA	-7.73	111.80	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	CYS	CA-C-N	-7.71	110.21	119.84
1	A	123	CYS	C-N-CA	-7.71	110.21	119.84
2	B	202	VAL	N-CA-C	7.45	119.81	108.71
2	B	154	GLY	CA-C-N	-7.41	112.13	119.76
2	B	154	GLY	C-N-CA	-7.41	112.13	119.76
1	D	123	CYS	CA-C-N	-7.40	110.59	119.84
1	D	123	CYS	C-N-CA	-7.40	110.59	119.84
2	E	202	VAL	N-CA-C	7.16	119.38	108.71
2	B	327	LEU	N-CA-C	-7.01	103.99	112.54
2	E	203	ILE	N-CA-C	-6.97	98.39	108.36
2	E	156	MET	CA-C-N	6.94	126.76	119.05
2	E	156	MET	C-N-CA	6.94	126.76	119.05
1	D	77	CYS	N-CA-C	6.83	118.72	111.28
2	E	327	LEU	N-CA-C	-6.68	104.07	111.82
1	D	43	GLY	N-CA-C	-6.60	103.62	112.14
2	E	127	THR	N-CA-C	-6.59	105.20	113.18
2	E	139	GLU	N-CA-C	6.56	119.76	111.69
2	B	156	MET	CA-C-N	6.52	126.75	119.32
2	B	156	MET	C-N-CA	6.52	126.75	119.32
2	E	24	ALA	N-CA-C	-6.49	99.45	109.76
1	A	77	CYS	N-CA-C	6.45	118.39	111.36
1	A	139	GLY	N-CA-C	6.43	128.42	113.18
2	E	341	VAL	N-CA-C	6.39	117.27	108.84
2	E	133	ILE	N-CA-C	6.34	118.98	111.05
2	E	150	ASP	CA-C-N	-6.34	113.61	119.82
2	E	150	ASP	C-N-CA	-6.34	113.61	119.82
1	D	279	ILE	N-CA-C	-6.21	104.80	110.82
2	E	272	THR	N-CA-C	-6.21	104.14	111.03
2	B	140	THR	CA-C-N	6.19	125.89	119.82
2	B	140	THR	C-N-CA	6.19	125.89	119.82
1	A	131	GLU	N-CA-C	6.17	121.00	111.56
1	D	70	ILE	N-CA-C	6.13	116.69	107.80
1	D	139	GLY	N-CA-C	6.13	127.72	113.18
2	B	195	LEU	N-CA-C	6.13	118.48	108.55
1	D	24	SER	N-CA-C	-6.13	104.16	111.69
2	E	321	GLY	N-CA-C	-6.12	103.75	112.81
1	A	149	ILE	N-CA-C	5.99	116.50	107.75
2	E	131	VAL	CA-C-N	-5.99	112.62	121.24
2	E	131	VAL	C-N-CA	-5.99	112.62	121.24
2	B	121	VAL	N-CA-C	-5.93	101.06	108.89
2	B	24	ALA	N-CA-C	-5.91	100.36	109.76
2	B	286	PHE	N-CA-C	-5.90	98.78	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	LYS	N-CA-C	5.83	118.66	109.39
1	A	43	GLY	N-CA-C	-5.76	105.31	111.93
2	E	105	ALA	N-CA-C	-5.71	103.82	112.04
1	A	24	SER	N-CA-C	-5.68	104.70	111.69
1	A	33	LYS	N-CA-C	5.65	118.38	109.39
1	A	87	ALA	CA-C-N	-5.65	115.45	123.08
1	A	87	ALA	C-N-CA	-5.65	115.45	123.08
2	E	343	VAL	N-CA-C	5.63	115.37	109.01
2	B	380	GLN	N-CA-C	5.62	117.08	111.07
2	B	203	ILE	N-CA-C	-5.60	100.35	108.36
2	E	195	LEU	N-CA-C	5.57	117.73	108.99
2	B	272	THR	N-CA-C	-5.56	104.91	110.97
2	E	161	ARG	N-CA-C	-5.47	105.40	111.36
2	B	150	ASP	CA-C-N	-5.44	114.08	120.12
2	B	150	ASP	C-N-CA	-5.44	114.08	120.12
2	E	121	VAL	N-CA-C	-5.43	101.72	108.89
2	B	207	GLY	N-CA-C	5.42	123.97	114.76
1	A	70	ILE	N-CA-C	5.41	115.65	107.80
2	E	380	GLN	N-CA-C	5.40	116.85	111.07
1	D	10	VAL	N-CA-C	5.39	115.66	108.11
1	A	137	GLN	N-CA-C	5.37	118.58	109.87
1	A	128	THR	CA-C-N	5.36	126.54	119.84
1	A	128	THR	C-N-CA	5.36	126.54	119.84
1	D	137	GLN	CA-C-N	5.36	126.54	119.84
1	D	137	GLN	C-N-CA	5.36	126.54	119.84
1	A	36	GLY	N-CA-C	5.36	118.29	110.63
1	A	175	VAL	N-CA-C	5.26	115.42	107.75
1	D	149	ILE	N-CA-C	5.23	115.43	108.11
2	B	356	LEU	N-CA-C	-5.22	105.71	111.71
1	D	131	GLU	N-CA-C	5.22	119.54	111.56
1	D	128	THR	CA-C-N	5.14	126.26	119.84
1	D	128	THR	C-N-CA	5.14	126.26	119.84
1	A	240	LYS	N-CA-C	5.13	117.48	110.55
2	B	96	ILE	N-CA-C	-5.12	100.94	108.11
1	A	279	ILE	N-CA-C	-5.11	105.86	110.82
1	D	36	GLY	N-CA-C	5.08	117.46	110.56
2	E	87	ASP	N-CA-C	-5.08	104.17	110.41
1	A	69	VAL	CB-CA-C	5.05	118.11	110.63
2	E	358	ALA	N-CA-C	-5.04	105.98	111.82
2	B	250	LEU	N-CA-C	-5.04	101.71	109.52
2	E	207	GLY	N-CA-C	5.03	123.31	114.76
1	A	14	GLY	N-CA-C	-5.03	106.83	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	GLN	CA-C-N	5.02	126.11	119.84
1	A	137	GLN	C-N-CA	5.02	126.11	119.84
1	D	283	LEU	N-CA-C	-5.02	105.89	111.36
2	E	65	SER	N-CA-C	5.01	117.00	109.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2069	0	2129	115	0
1	D	2069	0	2129	127	0
2	B	2904	0	2961	144	0
2	E	2881	0	2939	130	0
3	A	5	0	0	1	0
3	D	5	0	0	2	0
4	A	42	0	24	2	0
4	B	17	0	18	2	0
4	D	42	0	24	2	0
4	E	8	0	7	2	0
5	B	10	0	0	1	0
5	E	10	0	0	0	0
6	A	57	0	0	3	0
6	B	46	0	0	3	0
6	D	34	0	0	2	0
6	E	56	0	0	5	0
All	All	10255	0	10231	491	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 24.

All (491) 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)
2:E:369:ILE:HG22	2:E:370:ALA:H	1.23	1.04
2:B:369:ILE:HG22	2:B:370:ALA:H	1.25	0.98
2:E:295:LYS:HG2	2:E:331:GLY:HA2	1.46	0.97
2:B:295:LYS:HG2	2:B:331:GLY:HA2	1.46	0.94
1:A:145:GLY:HA3	1:A:170:GLY:HA3	1.51	0.89
1:D:145:GLY:HA3	1:D:170:GLY:HA3	1.54	0.88
2:B:291:GLY:O	2:B:293:ALA:N	2.08	0.85
1:D:117:ARG:HD3	1:D:193:MET:HE1	1.62	0.81
2:E:238:GLU:HG3	6:E:1928:HOH:O	1.79	0.81
1:A:117:ARG:HD3	1:A:193:MET:HE1	1.62	0.81
2:E:369:ILE:HG22	2:E:370:ALA:N	1.92	0.81
1:D:139:GLY:HA2	1:D:142:HIS:ND1	1.96	0.81
2:B:369:ILE:HG22	2:B:370:ALA:N	1.92	0.80
2:E:308:ASP:OD1	2:E:310:LYS:HG2	1.82	0.80
2:B:343:VAL:HG12	2:B:344:PRO:HD2	1.63	0.79
2:B:310:LYS:HE3	6:B:1936:HOH:O	1.82	0.79
2:E:325:CYS:HB2	2:E:352:ASN:O	1.81	0.79
2:E:343:VAL:HB	2:E:344:PRO:HD2	1.62	0.78
2:B:325:CYS:HB2	2:B:352:ASN:O	1.83	0.78
1:A:169:PHE:CE1	1:A:287:LEU:HD23	2.18	0.78
1:A:139:GLY:HA2	1:A:142:HIS:ND1	1.99	0.77
2:E:369:ILE:HG21	2:E:380:GLN:OE1	1.86	0.76
1:D:124:PRO:HB2	1:D:176:GLY:O	1.85	0.76
2:B:369:ILE:CG2	2:B:370:ALA:H	1.99	0.75
2:E:64:ASN:ND2	6:E:1924:HOH:O	2.19	0.75
2:B:308:ASP:OD1	2:B:310:LYS:HG2	1.86	0.75
1:D:223:GLU:HG2	1:D:224:HIS:CD2	2.22	0.75
1:A:124:PRO:HB2	1:A:176:GLY:O	1.86	0.74
2:E:75:ASN:O	2:E:79:LYS:HD2	1.87	0.73
2:B:36:SER:HB2	6:D:1630:HOH:O	1.87	0.72
1:A:223:GLU:HG2	1:A:224:HIS:CD2	2.24	0.72
1:A:129:PRO:HG2	1:A:171:GLN:HB2	1.70	0.71
2:B:348:ARG:C	2:B:348:ARG:HD2	2.16	0.71
1:D:129:PRO:HG2	1:D:171:GLN:HB2	1.72	0.71
2:E:369:ILE:CG2	2:E:370:ALA:H	2.00	0.71
1:D:273:VAL:CG2	1:D:278:ASP:HB2	2.20	0.71
2:B:315:LEU:HB2	2:B:381:VAL:HG11	1.73	0.71
1:A:186:ASN:HD22	1:A:187:PHE:H	1.39	0.70
2:E:103:ASP:HB3	2:E:205:LYS:HG3	1.74	0.70
2:B:302:PHE:CE1	2:B:314:VAL:HG11	2.27	0.70
2:B:279:HIS:O	2:B:382:VAL:HG11	1.92	0.69
2:B:369:ILE:HG21	2:B:380:GLN:OE1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:PHE:CE1	1:D:287:LEU:HD23	2.27	0.69
1:A:273:VAL:HG23	1:A:278:ASP:HB2	1.75	0.69
2:E:258:ASN:H	2:E:258:ASN:HD22	1.39	0.69
2:E:315:LEU:HB2	2:E:381:VAL:HG11	1.72	0.68
1:D:273:VAL:HG23	1:D:278:ASP:HB2	1.75	0.68
2:B:75:ASN:O	2:B:79:LYS:HD2	1.93	0.67
2:B:103:ASP:HB3	2:B:205:LYS:HG3	1.76	0.67
2:E:279:HIS:O	2:E:382:VAL:HG11	1.95	0.67
1:A:39:THR:HG21	1:A:42:LYS:HD2	1.76	0.67
1:A:23:HIS:CD2	1:A:136:ILE:HG22	2.31	0.66
1:D:159:GLU:OE2	2:E:319:PHE:CD2	2.48	0.66
1:A:155:THR:HG21	2:B:264:ASN:O	1.95	0.66
1:A:273:VAL:CG2	1:A:278:ASP:HB2	2.25	0.66
1:D:23:HIS:CG	1:D:136:ILE:HG22	2.31	0.66
1:D:186:ASN:HD22	1:D:187:PHE:H	1.42	0.66
1:D:285:THR:HG22	1:D:286:VAL:N	2.10	0.66
1:A:273:VAL:HG13	1:A:273:VAL:O	1.95	0.65
2:B:294:THR:O	2:B:298:VAL:HG23	1.96	0.65
2:E:325:CYS:O	2:E:349:LEU:HD13	1.97	0.65
1:D:273:VAL:HG13	1:D:273:VAL:O	1.95	0.65
2:E:383:ALA:O	2:E:385:VAL:N	2.30	0.65
1:D:9:LYS:HD3	1:D:35:VAL:HG11	1.78	0.64
2:E:296:GLU:CD	2:E:296:GLU:H	2.05	0.64
1:A:23:HIS:CG	1:A:136:ILE:HG22	2.31	0.64
2:E:294:THR:O	2:E:298:VAL:HG23	1.97	0.64
1:A:124:PRO:CB	1:A:176:GLY:O	2.45	0.64
2:B:325:CYS:O	2:B:349:LEU:HD13	1.97	0.64
1:D:197:ASP:O	1:D:227:LYS:NZ	2.31	0.64
2:B:229:LEU:HA	2:B:232:MET:HE3	1.79	0.64
2:E:348:ARG:HD2	2:E:348:ARG:C	2.22	0.64
1:A:150:VAL:CG1	1:A:190:ILE:HG21	2.29	0.63
2:B:371:ALA:CB	2:B:377:ALA:HB2	2.28	0.63
1:D:23:HIS:CD2	1:D:136:ILE:HG22	2.33	0.63
1:D:42:LYS:NZ	4:D:1301:COA:O7A	2.31	0.63
1:A:275:SER:HB2	2:B:278:LEU:HD21	1.80	0.63
2:B:70:ARG:O	2:B:74:GLU:HG3	1.99	0.63
2:E:302:PHE:CE1	2:E:314:VAL:HG11	2.33	0.63
1:D:81:ILE:O	1:D:85:ILE:HG13	1.99	0.62
2:B:292:GLY:O	2:B:294:THR:N	2.28	0.62
1:D:124:PRO:CB	1:D:176:GLY:O	2.48	0.62
1:A:222:LYS:HB2	1:A:268:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:ASN:HD22	2:B:258:ASN:H	1.44	0.62
1:D:222:LYS:HB2	1:D:268:ALA:HB1	1.82	0.62
2:B:383:ALA:O	2:B:385:VAL:N	2.32	0.62
2:E:124:MET:HA	2:E:145:HIS:O	2.00	0.61
1:D:237:THR:HG23	2:E:274:ASP:OD1	1.99	0.61
1:D:39:THR:HG21	1:D:42:LYS:HD2	1.82	0.61
2:E:70:ARG:O	2:E:74:GLU:HG3	2.00	0.61
2:E:87:ASP:C	2:E:87:ASP:OD1	2.42	0.61
1:D:93:ILE:HD12	1:D:126:VAL:HG23	1.82	0.61
1:A:138:PRO:O	1:A:141:ILE:HG12	2.00	0.61
1:A:285:THR:HG22	1:A:286:VAL:N	2.16	0.61
2:B:296:GLU:CD	2:B:296:GLU:H	2.08	0.60
1:A:275:SER:HB2	2:B:278:LEU:CD2	2.31	0.60
1:A:276:LEU:H	1:A:276:LEU:HD23	1.66	0.60
1:A:281:GLU:O	1:A:284:LYS:HB3	2.02	0.60
1:A:164:THR:HG22	1:A:283:LEU:HD12	1.84	0.60
1:D:138:PRO:O	1:D:141:ILE:HG12	2.02	0.60
1:D:156:LEU:HD11	1:D:234:ALA:HB2	1.84	0.60
1:A:156:LEU:HG	2:B:267:GLY:C	2.27	0.59
2:E:371:ALA:CB	2:E:377:ALA:HB2	2.32	0.59
2:B:87:ASP:C	2:B:87:ASP:OD1	2.46	0.59
1:D:164:THR:HG22	1:D:283:LEU:HD12	1.83	0.59
1:D:159:GLU:OE2	2:E:319:PHE:HD2	1.84	0.59
1:A:166:ASP:C	1:A:168:GLY:H	2.11	0.58
2:B:124:MET:HE3	2:B:146:LYS:HE2	1.85	0.58
1:D:240:LYS:HG2	1:D:251:ILE:HG21	1.86	0.58
2:B:348:ARG:NH1	2:B:348:ARG:HG3	2.18	0.58
1:D:248:GLY:O	2:E:116:ARG:NH2	2.36	0.58
1:A:156:LEU:HD11	1:A:234:ALA:HB2	1.85	0.58
1:D:281:GLU:O	1:D:284:LYS:HB3	2.03	0.58
1:A:240:LYS:HG2	1:A:251:ILE:HG21	1.86	0.58
1:D:169:PHE:HZ	1:D:284:LYS:HA	1.70	0.57
2:E:318:ILE:HG22	2:E:319:PHE:N	2.19	0.57
1:A:151:SER:HB2	1:A:206:ILE:HB	1.85	0.57
2:B:229:LEU:HD23	2:B:232:MET:HE3	1.86	0.57
2:B:233:ARG:NH2	5:B:1500:SO4:O4	2.37	0.57
2:E:248:TRP:CD2	2:E:300:GLU:HG3	2.39	0.57
1:A:30:TYR:O	1:A:30:TYR:CD1	2.57	0.57
2:B:385:VAL:O	2:B:388:LYS:HG3	2.04	0.57
2:B:310:LYS:HG3	6:B:1936:HOH:O	2.05	0.57
1:A:81:ILE:O	1:A:85:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:17:LEU:N	2:E:17:LEU:HD23	2.19	0.57
1:A:197:ASP:O	1:A:227:LYS:NZ	2.38	0.56
2:E:35:ALA:HB2	2:E:69:ILE:CD1	2.35	0.56
2:B:248:TRP:CD2	2:B:300:GLU:HG3	2.40	0.56
1:D:192:GLU:HG3	1:D:220:TYR:OH	2.04	0.56
1:A:192:GLU:HG3	1:A:220:TYR:OH	2.05	0.56
1:A:199:GLN:O	1:A:199:GLN:HG3	2.04	0.56
1:D:6:LYS:N	1:D:131:GLU:HB3	2.21	0.56
2:E:361:LEU:HD22	2:E:368:ILE:HG21	1.86	0.56
1:D:4:ILE:HD12	1:D:132:CYS:HB3	1.88	0.56
1:D:150:VAL:CG1	1:D:190:ILE:HG21	2.36	0.56
1:D:155:THR:HG21	2:E:264:ASN:O	2.06	0.56
1:A:123:CYS:SG	4:A:1300:COA:C6P	2.94	0.56
1:D:67:ALA:HA	1:D:91:LEU:O	2.06	0.56
1:D:93:ILE:HD12	1:D:126:VAL:CG2	2.36	0.55
1:A:181:PRO:HB2	2:B:116:ARG:HD3	1.88	0.55
1:A:164:THR:HG22	1:A:283:LEU:CD1	2.35	0.55
2:B:249:GLU:OE1	2:E:70:ARG:NH2	2.39	0.55
2:B:348:ARG:HG3	2:B:348:ARG:HH11	1.71	0.55
2:E:258:ASN:H	2:E:258:ASN:ND2	2.03	0.55
1:D:32:THR:HG23	1:D:132:CYS:SG	2.47	0.55
1:D:95:ILE:HA	1:D:124:PRO:HD2	1.87	0.55
1:A:57:ARG:NH1	1:A:86:ASP:O	2.40	0.55
1:D:11:ILE:HA	1:D:36:GLY:O	2.07	0.55
2:E:348:ARG:HH12	2:E:374:LEU:HB2	1.71	0.55
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.89	0.55
2:B:258:ASN:H	2:B:258:ASN:ND2	2.04	0.55
2:B:3:LEU:HD12	2:B:216:LEU:HB2	1.88	0.55
2:E:191:ARG:HB3	2:E:229:LEU:HD11	1.89	0.55
1:A:95:ILE:HA	1:A:124:PRO:HD2	1.89	0.55
1:A:203:ILE:HB	1:A:229:VAL:HG22	1.89	0.55
2:B:35:ALA:HB2	2:B:69:ILE:CD1	2.36	0.55
2:B:87:ASP:OD1	2:B:89:ASN:N	2.38	0.55
2:B:340:GLY:O	2:B:342:ASN:OD1	2.24	0.55
1:D:142:HIS:CD2	1:D:161:VAL:HG11	2.42	0.55
1:D:203:ILE:HB	1:D:229:VAL:HG22	1.88	0.55
1:A:109:VAL:O	1:A:113:GLU:HG2	2.06	0.55
2:B:369:ILE:HD12	2:B:369:ILE:N	2.22	0.54
2:E:359:LYS:O	2:E:360:LYS:C	2.50	0.54
1:A:6:LYS:N	1:A:131:GLU:HB3	2.22	0.54
1:A:154:GLY:O	1:A:157:THR:HB	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:LEU:HD23	2:B:232:MET:CE	2.37	0.54
2:E:125:ALA:HB1	2:E:167:LEU:HD11	1.88	0.54
1:A:9:LYS:HD3	1:A:35:VAL:HG11	1.89	0.54
1:A:169:PHE:HZ	1:A:284:LYS:HA	1.73	0.54
1:D:246:HIS:NE2	3:D:1601:PO4:O2	2.40	0.54
2:B:263:VAL:HG12	2:B:264:ASN:N	2.23	0.54
2:B:302:PHE:HE1	2:B:314:VAL:HG11	1.72	0.54
1:D:164:THR:HG22	1:D:283:LEU:CD1	2.37	0.54
1:A:186:ASN:ND2	1:A:187:PHE:H	2.06	0.54
2:B:318:ILE:HG22	2:B:319:PHE:N	2.23	0.54
2:B:125:ALA:HB1	2:B:167:LEU:HD11	1.89	0.53
2:E:229:LEU:HD23	2:E:232:MET:CE	2.39	0.53
1:A:42:LYS:NZ	4:A:1300:COA:O7A	2.40	0.53
1:D:146:LYS:HG2	1:D:169:PHE:O	2.08	0.53
1:D:151:SER:HB3	1:D:157:THR:OG1	2.07	0.53
2:E:87:ASP:OD1	2:E:89:ASN:N	2.38	0.53
2:E:229:LEU:HD23	2:E:232:MET:HE3	1.89	0.53
2:E:343:VAL:HB	2:E:344:PRO:CD	2.38	0.53
2:B:359:LYS:O	2:B:361:LEU:N	2.41	0.53
1:D:30:TYR:O	1:D:30:TYR:CD1	2.61	0.53
2:E:328:ILE:O	2:E:332:ILE:HG13	2.08	0.53
2:E:325:CYS:SG	2:E:349:LEU:HB3	2.48	0.53
1:A:137:GLN:HB2	1:A:138:PRO:HD2	1.90	0.53
1:A:145:GLY:HA3	1:A:170:GLY:CA	2.31	0.53
2:B:17:LEU:N	2:B:17:LEU:HD23	2.23	0.53
1:A:146:LYS:HG2	1:A:169:PHE:O	2.08	0.53
2:B:141:PRO:HG2	6:B:1948:HOH:O	2.08	0.53
1:D:166:ASP:C	1:D:168:GLY:H	2.17	0.53
1:D:276:LEU:HD23	1:D:276:LEU:H	1.72	0.53
1:A:93:ILE:HD12	1:A:126:VAL:HG23	1.91	0.52
1:D:186:ASN:ND2	1:D:187:PHE:H	2.07	0.52
1:D:199:GLN:O	1:D:199:GLN:HG3	2.09	0.52
2:E:348:ARG:HG3	2:E:348:ARG:NH1	2.24	0.52
2:B:359:LYS:O	2:B:360:LYS:C	2.52	0.52
1:A:248:GLY:O	2:B:116:ARG:NH2	2.42	0.52
2:B:149:LEU:HD22	2:B:155:PRO:HB3	1.90	0.52
1:D:137:GLN:HB2	1:D:138:PRO:HD2	1.90	0.52
2:E:248:TRP:CE2	2:E:300:GLU:HG3	2.44	0.52
1:A:186:ASN:HD22	1:A:187:PHE:N	2.08	0.52
1:D:236:VAL:HA	1:D:258:ALA:HB3	1.92	0.52
2:E:372:LYS:HG3	6:E:1930:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HD12	1:A:132:CYS:HB3	1.90	0.52
1:A:150:VAL:HG11	1:A:190:ILE:HB	1.92	0.52
1:D:145:GLY:HA3	1:D:170:GLY:CA	2.33	0.52
2:B:348:ARG:HH11	2:B:348:ARG:CG	2.23	0.52
2:E:263:VAL:HG12	2:E:264:ASN:N	2.25	0.52
2:E:263:VAL:HG11	2:E:268:LEU:HG	1.92	0.52
2:E:359:LYS:O	2:E:361:LEU:N	2.42	0.52
2:B:263:VAL:HG11	2:B:268:LEU:HG	1.92	0.52
1:A:246:HIS:HB2	1:A:249:ALA:HB2	1.92	0.51
2:B:332:ILE:O	2:B:336:VAL:HG23	2.10	0.51
1:D:273:VAL:HG21	1:D:278:ASP:C	2.35	0.51
2:E:51:ALA:CB	2:E:86:THR:HG23	2.40	0.51
1:D:150:VAL:HG11	1:D:190:ILE:HB	1.91	0.51
1:D:191:LEU:HD13	1:D:221:ILE:HG13	1.93	0.51
2:E:35:ALA:HB2	2:E:69:ILE:HD12	1.93	0.51
1:A:153:SER:OG	2:B:267:GLY:HA3	2.11	0.51
1:A:273:VAL:HG21	1:A:278:ASP:C	2.36	0.51
2:B:295:LYS:HG2	2:B:331:GLY:CA	2.32	0.51
2:E:3:LEU:HD12	2:E:216:LEU:HB2	1.93	0.51
2:E:330:ASP:OD1	2:E:360:LYS:HD2	2.11	0.51
1:D:186:ASN:HD22	1:D:187:PHE:N	2.09	0.51
1:D:240:LYS:HG2	1:D:251:ILE:CG2	2.40	0.51
2:B:248:TRP:CE2	2:B:300:GLU:HG3	2.45	0.50
1:D:273:VAL:HG21	1:D:278:ASP:HB2	1.93	0.50
2:B:328:ILE:O	2:B:332:ILE:HG13	2.11	0.50
2:E:320:GLY:HA2	4:E:1904:COA:H32	1.94	0.50
1:D:146:LYS:HD2	1:D:287:LEU:HD21	1.94	0.50
2:E:383:ALA:C	2:E:385:VAL:H	2.19	0.50
2:B:383:ALA:C	2:B:385:VAL:H	2.19	0.50
2:E:258:ASN:ND2	2:E:259:ILE:HG13	2.26	0.50
1:A:150:VAL:CG1	1:A:190:ILE:CG2	2.90	0.50
1:A:236:VAL:HA	1:A:258:ALA:HB3	1.93	0.50
1:D:42:LYS:O	1:D:52:VAL:HG12	2.12	0.50
2:B:258:ASN:ND2	2:B:259:ILE:HG13	2.27	0.50
2:E:346:VAL:HB	2:E:381:VAL:CG1	2.42	0.49
1:D:154:GLY:O	1:D:157:THR:HB	2.11	0.49
2:B:348:ARG:HH12	2:B:374:LEU:HB2	1.78	0.49
2:B:51:ALA:CB	2:B:86:THR:HG23	2.42	0.49
2:B:64:ASN:H	2:B:64:ASN:ND2	2.10	0.49
2:B:346:VAL:HB	2:B:381:VAL:HG13	1.94	0.49
2:E:369:ILE:CG2	2:E:370:ALA:N	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:O	1:A:193:MET:HG3	2.12	0.49
2:E:369:ILE:HD12	2:E:369:ILE:N	2.27	0.49
2:E:332:ILE:O	2:E:336:VAL:HG23	2.13	0.49
1:D:123:CYS:O	1:D:124:PRO:O	2.29	0.49
1:A:151:SER:HB3	1:A:157:THR:OG1	2.12	0.49
1:A:246:HIS:NE2	3:A:1600:PO4:O2	2.46	0.49
1:A:169:PHE:CD1	1:A:287:LEU:HD23	2.47	0.49
2:B:254:ALA:C	2:B:255:LEU:HD12	2.38	0.49
2:B:272:THR:O	2:B:275:ILE:HG22	2.12	0.49
2:B:335:ALA:O	2:B:339:VAL:HB	2.13	0.49
2:E:91:GLN:NE2	2:E:237:GLN:O	2.40	0.48
1:A:273:VAL:O	1:A:273:VAL:CG1	2.62	0.48
1:D:189:ASP:O	1:D:193:MET:HG3	2.14	0.48
1:D:12:CYS:HB2	1:D:34:MET:HE1	1.95	0.48
2:E:119:ARG:HG3	2:E:119:ARG:HH11	1.77	0.48
2:E:254:ALA:C	2:E:255:LEU:HD12	2.37	0.48
2:B:84:TYR:CE1	2:B:85:GLN:HG3	2.48	0.48
2:B:140:THR:HB	2:B:143:LEU:HD12	1.95	0.48
2:E:229:LEU:HA	2:E:232:MET:HE3	1.94	0.48
1:A:273:VAL:HG22	1:A:275:SER:O	2.14	0.48
2:B:346:VAL:HB	2:B:381:VAL:CG1	2.43	0.48
1:D:147:VAL:CG1	1:D:204:VAL:HG23	2.44	0.48
1:A:240:LYS:HG2	1:A:251:ILE:CG2	2.43	0.48
2:B:361:LEU:HD22	2:B:368:ILE:HG21	1.96	0.48
1:D:109:VAL:O	1:D:113:GLU:HG2	2.13	0.48
1:D:151:SER:HB2	1:D:206:ILE:HB	1.96	0.48
2:E:245:ALA:HB1	2:E:250:LEU:HB2	1.96	0.48
2:E:348:ARG:HG3	2:E:348:ARG:HH11	1.78	0.48
1:D:285:THR:O	1:D:287:LEU:N	2.47	0.48
1:D:156:LEU:CD2	1:D:276:LEU:HD13	2.43	0.47
1:D:156:LEU:HG	2:E:267:GLY:C	2.39	0.47
1:D:201:GLU:O	1:D:228:PRO:HD2	2.13	0.47
1:D:253:GLY:HA2	2:E:134:GLU:OE1	2.13	0.47
1:A:67:ALA:HA	1:A:91:LEU:O	2.14	0.47
1:A:172:SER:HB3	1:A:199:GLN:HG2	1.96	0.47
2:E:256:ASP:O	2:E:257:GLY:O	2.32	0.47
2:B:315:LEU:HD12	2:B:316:VAL:N	2.29	0.47
2:E:378:ALA:O	2:E:382:VAL:HG23	2.15	0.47
1:D:223:GLU:HG2	1:D:224:HIS:NE2	2.29	0.47
2:B:374:LEU:C	2:B:376:ASP:N	2.72	0.47
2:E:64:ASN:ND2	2:E:64:ASN:H	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ARG:NH2	6:A:1619:HOH:O	2.34	0.47
2:B:336:VAL:HG13	2:B:341:VAL:HB	1.97	0.47
1:A:93:ILE:HD12	1:A:126:VAL:CG2	2.45	0.47
1:A:243:ARG:NE	6:A:1629:HOH:O	2.38	0.47
2:B:35:ALA:HB2	2:B:69:ILE:HD12	1.96	0.47
1:D:6:LYS:O	1:D:33:LYS:HE3	2.14	0.47
2:E:84:TYR:CE1	2:E:85:GLN:HG3	2.49	0.47
2:E:197:ALA:HB3	2:E:215:LYS:HB3	1.95	0.47
2:E:262:MET:HE1	2:E:302:PHE:CD2	2.49	0.47
2:E:324:ARG:O	2:E:326:ASP:N	2.48	0.47
2:E:346:VAL:HB	2:E:381:VAL:HG13	1.96	0.47
2:B:369:ILE:CG2	2:B:370:ALA:N	2.63	0.47
2:B:33:GLU:O	2:B:37:LYS:HG3	2.15	0.47
2:B:312:LYS:C	2:B:343:VAL:HG11	2.40	0.47
1:D:159:GLU:OE2	2:E:319:PHE:CE2	2.67	0.47
1:A:12:CYS:O	1:A:15:PHE:HB2	2.16	0.47
2:B:366:LEU:O	2:B:368:ILE:N	2.42	0.47
1:D:223:GLU:O	1:D:223:GLU:CG	2.63	0.46
1:A:167:TYR:C	1:A:169:PHE:H	2.23	0.46
1:D:159:GLU:OE2	2:E:348:ARG:NH2	2.48	0.46
2:E:235:GLN:O	2:E:238:GLU:HG2	2.15	0.46
2:B:324:ARG:O	2:B:326:ASP:N	2.49	0.46
2:E:272:THR:O	2:E:275:ILE:HG22	2.15	0.46
2:B:385:VAL:O	2:B:386:GLU:C	2.59	0.46
2:E:316:VAL:HB	2:E:347:VAL:HG22	1.96	0.46
2:E:359:LYS:O	2:E:362:ALA:N	2.48	0.46
2:B:197:ALA:HB3	2:B:215:LYS:HB3	1.97	0.46
2:B:318:ILE:HG21	2:B:328:ILE:CD1	2.45	0.46
1:D:3:LEU:HD21	1:D:193:MET:SD	2.54	0.46
2:E:272:THR:O	2:E:273:MET:C	2.58	0.46
1:A:221:ILE:HG22	1:A:222:LYS:N	2.30	0.46
1:D:127:ILE:HG22	1:D:174:CYS:HB2	1.96	0.46
1:A:123:CYS:O	1:A:124:PRO:O	2.34	0.46
1:A:166:ASP:C	1:A:168:GLY:N	2.72	0.46
2:B:156:MET:O	2:B:159:GLN:HB2	2.16	0.46
1:D:273:VAL:O	1:D:273:VAL:CG1	2.62	0.46
2:E:119:ARG:HG3	2:E:119:ARG:NH1	2.31	0.46
1:A:181:PRO:CB	2:B:116:ARG:HD3	2.46	0.46
2:B:292:GLY:O	2:B:294:THR:HG23	2.16	0.46
2:E:315:LEU:HD12	2:E:316:VAL:N	2.31	0.46
1:D:151:SER:CB	1:D:206:ILE:HB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:PRO:HB2	2:E:116:ARG:HD3	1.98	0.46
2:B:103:ASP:HB3	2:B:205:LYS:CG	2.44	0.45
2:B:124:MET:CE	2:B:146:LYS:HE2	2.46	0.45
1:A:142:HIS:CD2	1:A:161:VAL:HG11	2.51	0.45
1:A:277:ALA:CB	2:B:375:THR:HG23	2.46	0.45
2:B:133:ILE:O	2:B:133:ILE:HG13	2.17	0.45
2:E:5:GLU:OE2	2:E:9:LYS:NZ	2.49	0.45
2:E:32:GLU:O	6:E:1947:HOH:O	2.21	0.45
1:A:155:THR:OG1	2:B:268:LEU:HB2	2.16	0.45
2:B:140:THR:CB	2:B:143:LEU:HD12	2.47	0.45
2:B:290:GLY:O	2:B:291:GLY:C	2.59	0.45
2:E:348:ARG:HH11	2:E:348:ARG:CG	2.29	0.45
1:D:123:CYS:C	1:D:124:PRO:O	2.60	0.45
1:A:147:VAL:CG1	1:A:204:VAL:HG23	2.47	0.45
1:D:150:VAL:CG1	1:D:190:ILE:CG2	2.94	0.45
2:B:324:ARG:NH1	2:B:326:ASP:OD1	2.50	0.45
1:A:113:GLU:HG2	1:A:113:GLU:H	1.62	0.45
2:B:235:GLN:O	2:B:238:GLU:HG2	2.16	0.45
2:B:325:CYS:SG	2:B:349:LEU:HB3	2.56	0.45
2:E:199:ASN:HA	2:E:200:PRO:HA	1.76	0.45
2:B:359:LYS:O	2:B:362:ALA:N	2.50	0.44
2:B:1:MET:HE1	2:B:229:LEU:O	2.17	0.44
2:B:263:VAL:O	2:B:289:VAL:HG23	2.18	0.44
1:D:121:PRO:HG2	1:D:180:ASP:OD2	2.17	0.44
2:B:323:VAL:O	4:B:1903:COA:H22	2.16	0.44
1:A:223:GLU:O	1:A:223:GLU:CG	2.65	0.44
2:B:256:ASP:O	2:B:257:GLY:O	2.35	0.44
2:B:320:GLY:O	4:B:1903:COA:H21	2.18	0.44
2:B:32:GLU:OE2	2:B:70:ARG:NH1	2.51	0.44
1:D:98:GLY:HA2	2:E:221:ASN:ND2	2.33	0.44
1:D:275:SER:C	1:D:277:ALA:H	2.25	0.44
2:E:341:VAL:HG12	2:E:343:VAL:H	1.83	0.44
1:A:223:GLU:O	1:A:223:GLU:HG3	2.17	0.44
1:A:151:SER:CB	1:A:206:ILE:HB	2.47	0.44
1:D:195:GLU:CD	1:D:226:THR:H	2.25	0.44
2:E:239:ASP:OD1	2:E:239:ASP:C	2.60	0.44
2:B:10:GLN:O	2:B:13:ALA:HB3	2.18	0.44
1:D:167:TYR:C	1:D:169:PHE:H	2.26	0.43
1:A:164:THR:O	1:A:169:PHE:HB2	2.18	0.43
2:B:245:ALA:HB1	2:B:250:LEU:HB2	2.00	0.43
2:B:348:ARG:NH1	2:B:348:ARG:CG	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:GLU:O	2:E:37:LYS:HG3	2.19	0.43
2:B:239:ASP:OD1	2:B:239:ASP:C	2.59	0.43
1:D:57:ARG:NH1	1:D:86:ASP:O	2.52	0.43
2:E:256:ASP:OD1	2:E:256:ASP:N	2.39	0.43
2:E:257:GLY:HA3	2:E:282:GLU:O	2.18	0.43
1:A:285:THR:O	1:A:287:LEU:N	2.51	0.43
2:E:291:GLY:O	2:E:293:ALA:N	2.38	0.43
2:E:324:ARG:NH1	2:E:326:ASP:OD1	2.51	0.43
1:A:6:LYS:O	1:A:33:LYS:HE3	2.18	0.43
2:B:301:ALA:O	2:B:305:ILE:HG13	2.18	0.43
1:D:221:ILE:HG22	1:D:222:LYS:N	2.34	0.43
1:D:229:VAL:HG12	1:D:270:VAL:HG13	2.01	0.43
2:E:299:THR:OG1	2:E:335:ALA:HB2	2.19	0.43
1:A:223:GLU:HG2	1:A:224:HIS:NE2	2.34	0.43
1:D:57:ARG:HG3	1:D:87:ALA:CB	2.49	0.43
1:D:274:ARG:HA	1:D:274:ARG:HD3	1.78	0.43
1:A:133:LYS:NZ	1:A:137:GLN:O	2.45	0.43
1:D:246:HIS:HB2	1:D:249:ALA:HB2	2.01	0.43
2:E:258:ASN:HD22	2:E:258:ASN:N	2.03	0.43
1:A:15:PHE:CD2	1:A:37:GLY:HA3	2.53	0.43
1:A:155:THR:HB	2:B:268:LEU:HD22	1.99	0.43
1:A:158:TYR:CD1	1:A:158:TYR:N	2.87	0.43
2:B:313:ALA:HB2	2:B:385:VAL:HG13	2.00	0.43
2:E:219:ASP:OD1	2:E:221:ASN:HB2	2.18	0.43
2:E:374:LEU:C	2:E:376:ASP:N	2.76	0.43
1:A:156:LEU:CD2	1:A:276:LEU:HD13	2.49	0.43
1:A:191:LEU:HD13	1:A:221:ILE:HG13	2.00	0.43
2:B:20:PRO:HD3	2:B:211:CYS:O	2.18	0.43
2:B:312:LYS:O	2:B:385:VAL:HG12	2.19	0.43
1:D:99:ILE:HD12	1:D:121:PRO:CB	2.49	0.43
2:E:20:PRO:HD3	2:E:211:CYS:O	2.19	0.43
2:E:335:ALA:O	2:E:339:VAL:HB	2.19	0.43
1:D:246:HIS:NE2	3:D:1601:PO4:P	2.92	0.42
2:E:330:ASP:OD1	2:E:360:LYS:CD	2.67	0.42
2:B:272:THR:O	2:B:273:MET:C	2.61	0.42
1:D:123:CYS:O	1:D:124:PRO:C	2.62	0.42
1:D:227:LYS:HB3	1:D:228:PRO:HD2	2.00	0.42
2:E:149:LEU:HD22	2:E:155:PRO:HB3	2.00	0.42
2:E:172:LYS:HE3	2:E:207:GLY:O	2.19	0.42
1:A:273:VAL:HG22	1:A:275:SER:H	1.83	0.42
2:B:316:VAL:HB	2:B:347:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ARG:HG3	1:D:87:ALA:HB2	2.02	0.42
1:D:200:THR:O	1:D:227:LYS:HD3	2.20	0.42
1:D:223:GLU:O	1:D:223:GLU:HG3	2.19	0.42
2:E:1:MET:HE1	2:E:229:LEU:O	2.19	0.42
2:E:308:ASP:OD2	2:E:310:LYS:HG3	2.19	0.42
1:A:274:ARG:HD3	1:A:274:ARG:HA	1.79	0.42
2:B:15:TYR:CD1	2:B:187:ILE:HG12	2.54	0.42
2:B:282:GLU:HA	2:B:283:PRO:HD2	1.90	0.42
2:B:344:PRO:HG3	2:B:384:ALA:HB1	2.02	0.42
2:B:376:ASP:C	2:B:378:ALA:N	2.78	0.42
1:D:127:ILE:HG13	1:D:133:LYS:HB2	2.02	0.42
1:D:169:PHE:CD1	1:D:287:LEU:HD23	2.53	0.42
2:E:63:VAL:HB	6:E:1924:HOH:O	2.20	0.42
2:E:296:GLU:CD	2:E:296:GLU:N	2.77	0.42
1:A:167:TYR:HB2	1:A:169:PHE:CD2	2.55	0.42
1:D:71:TYR:C	4:D:1301:COA:H142	2.44	0.42
1:D:196:LYS:O	1:D:196:LYS:CG	2.68	0.42
2:E:235:GLN:HA	2:E:238:GLU:HG2	2.01	0.42
2:B:315:LEU:HD12	2:B:315:LEU:C	2.44	0.42
2:B:318:ILE:HG13	2:B:328:ILE:HD13	2.01	0.42
2:B:352:ASN:O	2:B:353:ASN:HB2	2.19	0.42
1:D:34:MET:HE3	1:D:34:MET:HB3	1.87	0.42
2:E:32:GLU:OE1	2:E:70:ARG:HD2	2.20	0.42
2:E:357:GLY:O	2:E:361:LEU:HG	2.20	0.42
1:A:123:CYS:C	1:A:124:PRO:O	2.62	0.41
1:D:221:ILE:HA	1:D:225:VAL:HG23	2.01	0.41
1:A:127:ILE:HG22	1:A:174:CYS:HB2	2.02	0.41
2:B:317:ASN:OD1	2:B:317:ASN:C	2.63	0.41
1:D:204:VAL:HA	1:D:230:VAL:O	2.19	0.41
2:E:273:MET:SD	2:E:286:PHE:HB2	2.60	0.41
1:D:285:THR:HG22	1:D:286:VAL:H	1.85	0.41
2:E:318:ILE:HG21	2:E:328:ILE:CD1	2.51	0.41
2:E:352:ASN:O	2:E:353:ASN:HB2	2.20	0.41
1:A:11:ILE:HG23	1:A:65:ALA:CB	2.50	0.41
1:A:94:THR:O	1:A:121:PRO:HA	2.20	0.41
1:A:143:LYS:O	1:A:144:PRO:C	2.64	0.41
1:A:200:THR:O	1:A:227:LYS:HD3	2.20	0.41
2:B:124:MET:HA	2:B:145:HIS:O	2.21	0.41
2:B:273:MET:SD	2:B:286:PHE:HB2	2.61	0.41
1:D:196:LYS:O	1:D:196:LYS:HG2	2.19	0.41
2:B:78:GLY:HA3	2:E:247:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:VAL:CG1	1:D:76:PHE:HB2	2.50	0.41
1:D:230:VAL:HG21	1:D:283:LEU:HD23	2.03	0.41
2:B:287:LEU:HD13	2:B:288:ASP:N	2.36	0.41
2:B:299:THR:OG1	2:B:335:ALA:HB2	2.20	0.41
1:D:94:THR:O	1:D:121:PRO:HA	2.20	0.41
1:D:136:ILE:HG12	6:D:1619:HOH:O	2.20	0.41
2:E:320:GLY:H	4:E:1904:COA:H21	1.85	0.41
1:A:199:GLN:O	1:A:199:GLN:CG	2.66	0.41
2:B:258:ASN:HD22	2:B:258:ASN:N	2.09	0.41
2:B:312:LYS:HG3	2:B:388:LYS:O	2.20	0.41
1:D:56:VAL:O	1:D:60:VAL:HG23	2.21	0.41
1:D:143:LYS:O	1:D:144:PRO:C	2.63	0.41
2:E:156:MET:HA	2:E:157:PRO:HD3	1.87	0.41
2:E:318:ILE:CG2	2:E:319:PHE:N	2.82	0.41
2:E:344:PRO:HG3	2:E:384:ALA:HB1	2.03	0.41
1:D:273:VAL:HG22	1:D:275:SER:H	1.86	0.41
2:B:355:GLU:C	2:B:357:GLY:N	2.77	0.40
1:D:2:ILE:O	1:D:4:ILE:N	2.46	0.40
1:D:158:TYR:CD1	1:D:158:TYR:N	2.87	0.40
1:A:146:LYS:HD2	1:A:287:LEU:HD21	2.01	0.40
1:A:159:GLU:OE2	2:B:348:ARG:NH2	2.54	0.40
2:B:32:GLU:CD	2:B:70:ARG:HH11	2.30	0.40
1:D:11:ILE:HG23	1:D:65:ALA:CB	2.51	0.40
1:A:5:ASP:HB2	1:A:131:GLU:OE1	2.20	0.40
2:B:212:LEU:HD12	2:B:212:LEU:HA	1.93	0.40
1:D:42:LYS:O	1:D:52:VAL:CG1	2.69	0.40
2:E:57:ALA:CB	2:E:83:THR:HG22	2.51	0.40
2:E:158:TYR:CD1	2:E:158:TYR:C	2.99	0.40
2:E:312:LYS:O	2:E:385:VAL:HG12	2.21	0.40
1:A:3:LEU:HD21	1:A:193:MET:SD	2.62	0.40
1:A:124:PRO:O	6:A:1655:HOH:O	2.21	0.40
1:A:246:HIS:HB2	1:A:249:ALA:CB	2.51	0.40
2:B:199:ASN:HA	2:B:200:PRO:HA	1.76	0.40
2:B:312:LYS:HA	2:B:312:LYS:HD3	1.84	0.40
2:B:369:ILE:N	2:B:369:ILE:CD1	2.85	0.40
1:D:142:HIS:CD2	1:D:161:VAL:CG1	3.04	0.40
1:A:201:GLU:O	1:A:228:PRO:HD2	2.21	0.40
2:B:256:ASP:OD1	2:B:256:ASP:N	2.39	0.40
2:E:31:ALA:O	2:E:34:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/288 (99%)	258 (90%)	21 (7%)	6 (2%)	5	15
1	D	285/288 (99%)	252 (88%)	27 (10%)	6 (2%)	5	15
2	B	386/388 (100%)	348 (90%)	27 (7%)	11 (3%)	4	9
2	E	383/388 (99%)	351 (92%)	25 (6%)	7 (2%)	6	18
All	All	1339/1352 (99%)	1209 (90%)	100 (8%)	30 (2%)	5	14

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	THR
2	B	292	GLY
2	B	293	ALA
2	B	384	ALA
1	D	285	THR
1	D	286	VAL
2	E	384	ALA
1	A	139	GLY
1	A	286	VAL
2	B	257	GLY
2	B	325	CYS
2	B	360	LYS
2	B	386	GLU
1	D	139	GLY
2	E	257	GLY
2	E	292	GLY
2	E	293	ALA
2	E	325	CYS
2	E	360	LYS
1	A	124	PRO
2	B	309	ASP
1	D	3	LEU

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Mol	Chain	Res	Type
1	D	124	PRO
2	B	139	GLU
2	B	291	GLY
1	D	138	PRO
1	A	3	LEU
1	A	138	PRO
2	B	369	ILE
2	E	369	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/218 (100%)	207 (95%)	10 (5%)	24	51
1	D	217/218 (100%)	206 (95%)	11 (5%)	21	48
2	B	297/297 (100%)	275 (93%)	22 (7%)	13	32
2	E	295/297 (99%)	271 (92%)	24 (8%)	11	27
All	All	1026/1030 (100%)	959 (94%)	67 (6%)	15	37

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	CYS
1	A	93	ILE
1	A	100	PRO
1	A	113	GLU
1	A	124	PRO
1	A	150	VAL
1	A	186	ASN
1	A	221	ILE
1	A	271	LYS
1	A	278	ASP
2	B	11	LEU
2	B	65	SER
2	B	70	ARG

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Mol	Chain	Res	Type
2	B	95	GLN
2	B	116	ARG
2	B	124	MET
2	B	139	GLU
2	B	195	LEU
2	B	200	PRO
2	B	202	VAL
2	B	256	ASP
2	B	258	ASN
2	B	287	LEU
2	B	288	ASP
2	B	300	GLU
2	B	323	VAL
2	B	327	LEU
2	B	328	ILE
2	B	343	VAL
2	B	348	ARG
2	B	369	ILE
2	B	375	THR
1	D	77	CYS
1	D	93	ILE
1	D	100	PRO
1	D	113	GLU
1	D	124	PRO
1	D	144	PRO
1	D	150	VAL
1	D	186	ASN
1	D	221	ILE
1	D	271	LYS
1	D	278	ASP
2	E	1	MET
2	E	11	LEU
2	E	64	ASN
2	E	65	SER
2	E	95	GLN
2	E	116	ARG
2	E	124	MET
2	E	138	GLU
2	E	146	LYS
2	E	195	LEU
2	E	200	PRO
2	E	256	ASP

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Mol	Chain	Res	Type
2	E	258	ASN
2	E	287	LEU
2	E	288	ASP
2	E	295	LYS
2	E	300	GLU
2	E	323	VAL
2	E	325	CYS
2	E	327	LEU
2	E	328	ILE
2	E	348	ARG
2	E	369	ILE
2	E	375	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
1	A	224	HIS
2	B	64	ASN
2	B	94	ASN
2	B	95	GLN
2	B	175	GLN
2	B	247	GLN
2	B	258	ASN
1	D	7	ASN
1	D	186	ASN
1	D	224	HIS
2	E	2	ASN
2	E	64	ASN
2	E	94	ASN
2	E	95	GLN
2	E	175	GLN
2	E	247	GLN
2	E	258	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	B	1500	-	4,4,4	0.49	0	6,6,6	0.25	0
4	COA	E	1904	2	6,7,50	1.85	2 (33%)	6,7,75	5.55	4 (66%)
3	PO4	A	1600	-	4,4,4	1.81	1 (25%)	6,6,6	0.51	0
5	SO4	E	1401	-	4,4,4	0.36	0	6,6,6	0.38	0
5	SO4	B	1400	-	4,4,4	0.37	0	6,6,6	0.54	0
5	SO4	E	1501	-	4,4,4	0.47	0	6,6,6	0.33	0
3	PO4	D	1601	-	4,4,4	1.68	1 (25%)	6,6,6	0.41	0
4	COA	A	1300	-	42,44,50	0.99	3 (7%)	62,68,75	1.62	10 (16%)
4	COA	D	1301	-	42,44,50	1.00	3 (7%)	62,68,75	1.68	10 (16%)
4	COA	B	1903	2	14,16,50	7.70	6 (42%)	19,21,75	4.49	15 (78%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	COA	A	1300	-	-	2/41/57/64	0/3/3/3
4	COA	E	1904	2	-	1/6/6/64	-
4	COA	D	1301	-	-	2/41/57/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	COA	B	1903	2	-	5/20/20/64	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1903	COA	CBP-CAP	27.72	1.73	1.55
4	B	1903	COA	C6P-C5P	3.70	1.58	1.51
4	B	1903	COA	C2P-S1P	3.53	1.94	1.80
4	E	1904	COA	C6P-C5P	3.15	1.61	1.51
4	B	1903	COA	C7P-N8P	3.05	1.53	1.46
4	B	1903	COA	C3P-N4P	2.97	1.52	1.46
4	A	1300	COA	P1A-O3A	2.82	1.62	1.59
4	D	1301	COA	P1A-O3A	2.62	1.62	1.59
3	A	1600	PO4	P-O2	-2.40	1.47	1.54
4	B	1903	COA	CCP-CBP	2.37	1.58	1.53
4	A	1300	COA	CCP-CBP	2.35	1.56	1.52
3	D	1601	PO4	P-O2	-2.26	1.48	1.54
4	D	1301	COA	CDP-CBP	-2.26	1.49	1.53
4	D	1301	COA	P2A-O3A	2.20	1.61	1.59
4	E	1904	COA	C2P-S1P	2.20	1.89	1.80
4	A	1300	COA	P2A-O3A	2.01	1.61	1.59

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1904	COA	C6P-C5P-N4P	10.27	126.64	115.75
4	B	1903	COA	CEP-CBP-CCP	-8.08	93.05	108.80
4	B	1903	COA	CAP-C9P-N8P	7.27	130.27	116.48
4	E	1904	COA	C3P-N4P-C5P	7.20	136.24	122.82
4	B	1903	COA	O5P-C5P-C6P	-6.64	109.98	122.02
4	B	1903	COA	C6P-C5P-N4P	6.61	128.39	116.34
4	A	1300	COA	CAP-C9P-N8P	6.14	128.14	116.48
4	D	1301	COA	CAP-C9P-N8P	6.07	128.00	116.48
4	B	1903	COA	OAP-CAP-CBP	-5.97	98.83	109.38
4	A	1300	COA	CEP-CBP-CAP	5.39	117.95	108.77
4	B	1903	COA	C6P-C7P-N8P	5.02	122.69	112.00
4	B	1903	COA	CEP-CBP-CAP	4.87	120.69	109.59
4	D	1301	COA	CEP-CBP-CCP	-4.56	100.70	108.22
4	B	1903	COA	C3P-N4P-C5P	4.22	130.68	122.82
4	E	1904	COA	O5P-C5P-C6P	-4.14	110.94	122.13
4	D	1301	COA	O9P-C9P-CAP	-4.13	109.37	120.89
4	B	1903	COA	CDP-CBP-CAP	4.10	118.94	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1301	COA	CEP-CBP-CAP	4.01	115.61	108.77
4	B	1903	COA	C7P-N8P-C9P	4.00	129.73	122.55
4	B	1903	COA	O9P-C9P-N8P	-3.95	114.61	122.98
4	D	1301	COA	CDP-CBP-CCP	3.77	114.45	108.22
4	A	1300	COA	CEP-CBP-CCP	-3.41	102.60	108.22
4	A	1300	COA	OAP-CAP-CBP	-3.18	102.80	110.18
4	E	1904	COA	C7P-C6P-C5P	3.16	123.67	113.29
4	D	1301	COA	C6P-C7P-N8P	3.09	121.81	111.53
4	D	1301	COA	O3B-P3B-O7A	-3.07	98.38	109.33
4	A	1300	COA	C6P-C7P-N8P	2.88	121.10	111.53
4	A	1300	COA	O9P-C9P-CAP	-2.88	112.86	120.89
4	D	1301	COA	OAP-CAP-CBP	-2.82	103.64	110.18
4	A	1300	COA	CDP-CBP-CCP	2.66	112.61	108.22
4	D	1301	COA	P2A-O6A-CCP	2.53	134.87	121.12
4	D	1301	COA	O6A-CCP-CBP	2.47	114.52	110.55
4	B	1903	COA	CEP-CBP-CDP	-2.44	104.04	108.80
4	A	1300	COA	P2A-O6A-CCP	2.37	134.01	121.12
4	B	1903	COA	C2P-C3P-N4P	2.33	117.60	112.31
4	B	1903	COA	OAP-CAP-C9P	-2.15	100.41	109.38
4	B	1903	COA	O9P-C9P-CAP	-2.08	115.08	120.89
4	A	1300	COA	CDP-CBP-CAP	-2.06	105.25	108.77
4	A	1300	COA	O4B-C1B-C2B	-2.02	102.30	106.62

There are no chirality outliers.

All (10) torsion outliers are listed below:

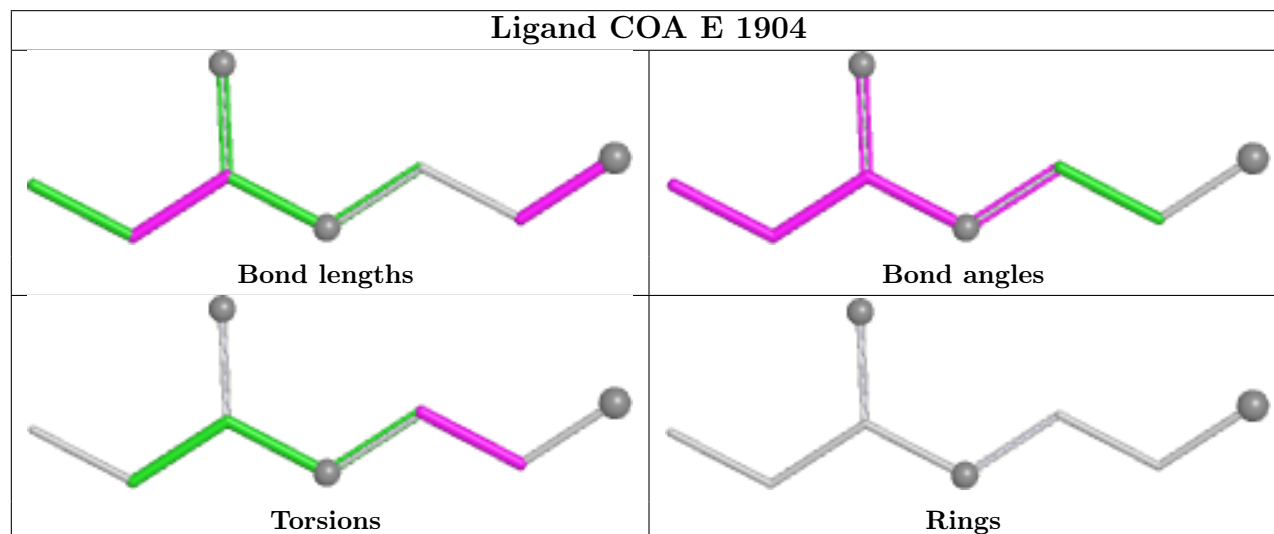
Mol	Chain	Res	Type	Atoms
4	B	1903	COA	N8P-C9P-CAP-OAP
4	B	1903	COA	S1P-C2P-C3P-N4P
4	E	1904	COA	S1P-C2P-C3P-N4P
4	B	1903	COA	O9P-C9P-CAP-OAP
4	B	1903	COA	O9P-C9P-CAP-CBP
4	B	1903	COA	N8P-C9P-CAP-CBP
4	A	1300	COA	C2B-C1B-N9A-C8A
4	D	1301	COA	C2B-C1B-N9A-C8A
4	D	1301	COA	O4B-C1B-N9A-C8A
4	A	1300	COA	N8P-C9P-CAP-OAP

There are no ring outliers.

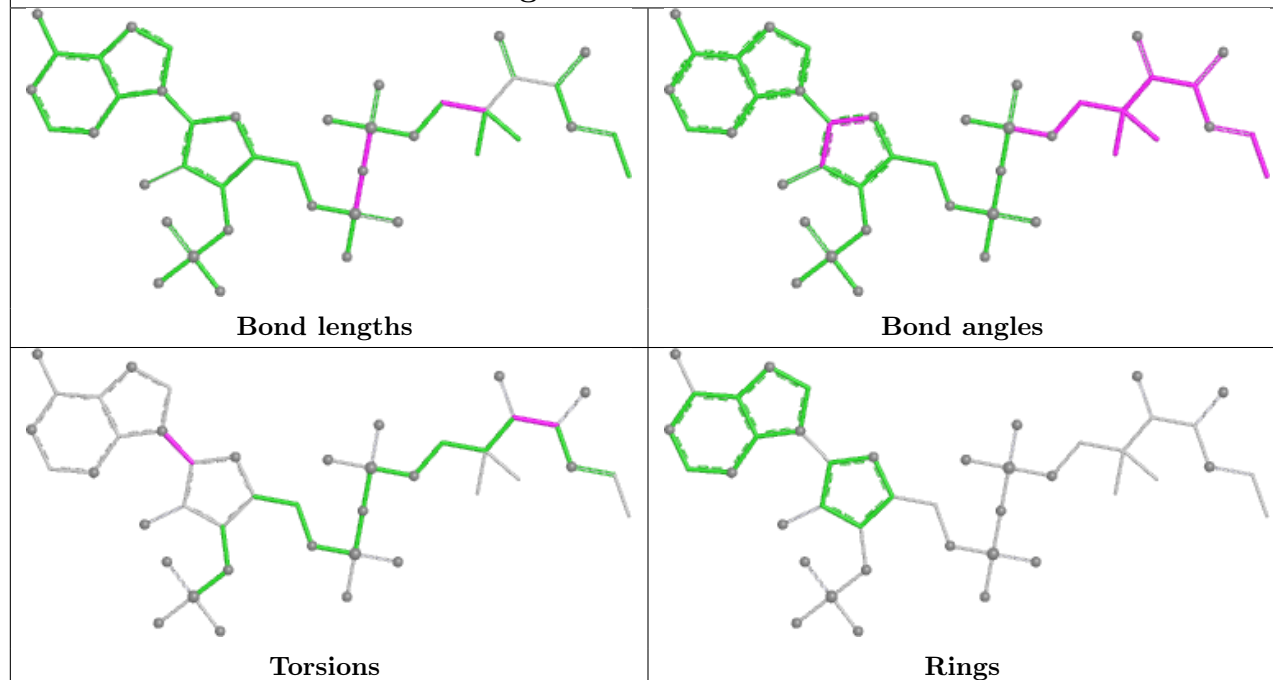
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1500	SO4	1	0
4	E	1904	COA	2	0
3	A	1600	PO4	1	0
3	D	1601	PO4	2	0
4	A	1300	COA	2	0
4	D	1301	COA	2	0
4	B	1903	COA	2	0

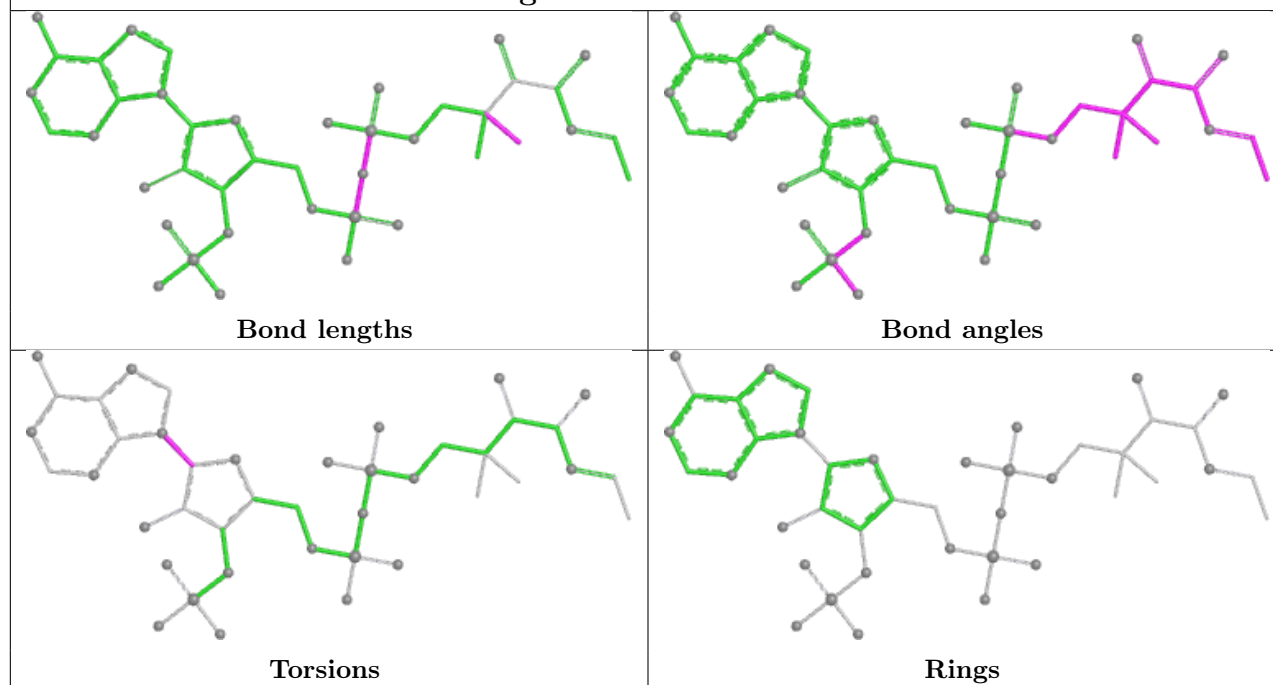
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

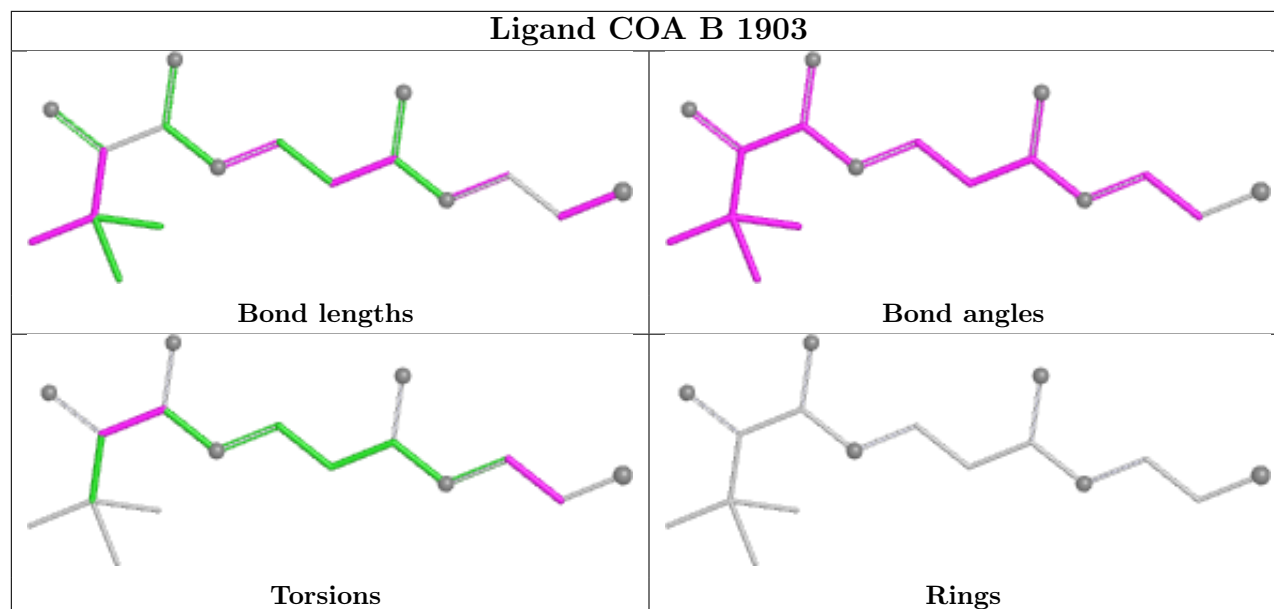


Ligand COA A 1300



Ligand COA D 1301





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	287/288 (99%)	0.01	8 (2%) 55 51	21, 42, 67, 82	0
1	D	287/288 (99%)	0.64	18 (6%) 26 23	29, 54, 78, 91	0
2	B	388/388 (100%)	0.36	43 (11%) 10 8	20, 48, 84, 96	0
2	E	385/388 (99%)	0.21	13 (3%) 48 44	25, 51, 79, 87	0
All	All	1347/1352 (99%)	0.30	82 (6%) 27 24	20, 49, 81, 96	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	GLY	5.9
2	B	339	VAL	4.5
2	E	384	ALA	4.4
1	D	139	GLY	4.4
2	B	313	ALA	3.9
1	D	270	VAL	3.9
2	B	357	GLY	3.9
1	D	136	ILE	3.8
2	B	291	GLY	3.7
2	E	373	GLY	3.5
2	B	336	VAL	3.4
2	B	258	ASN	3.3
2	B	337	ALA	3.3
2	B	372	LYS	3.3
2	B	354	ALA	3.3
2	B	295	LYS	3.2
1	D	282	ALA	3.2
2	B	361	LEU	3.1
2	B	358	ALA	3.1
2	B	338	GLU	3.1
2	B	290	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	7	ASN	3.1
2	E	363	ASP	3.0
2	B	335	ALA	3.0
2	B	370	ALA	3.0
2	B	278	LEU	2.9
2	B	375	THR	2.8
2	B	346	VAL	2.8
2	B	280	GLY	2.8
2	B	292	GLY	2.8
2	B	334	GLY	2.7
2	B	309	ASP	2.7
2	E	66	LYS	2.7
2	B	343	VAL	2.6
1	D	140	HIS	2.6
2	B	257	GLY	2.6
1	A	284	LYS	2.5
2	B	341	VAL	2.5
2	E	374	LEU	2.5
2	E	293	ALA	2.5
1	D	271	LYS	2.5
2	B	369	ILE	2.5
1	D	29	ALA	2.5
1	D	287	LEU	2.4
2	E	385	VAL	2.4
2	E	367	ASN	2.4
2	E	291	GLY	2.4
2	B	311	VAL	2.4
1	A	254	GLY	2.4
2	E	36	SER	2.3
2	E	369	ILE	2.3
2	B	312	LYS	2.3
1	D	36	GLY	2.3
2	B	384	ALA	2.3
1	A	255	LYS	2.3
1	D	186	ASN	2.3
2	B	248	TRP	2.3
2	B	281	GLY	2.3
1	D	283	LEU	2.3
1	D	202	ALA	2.2
2	E	132	GLU	2.2
2	B	385	VAL	2.2
2	B	322	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	259	ASP	2.2
2	B	327	LEU	2.2
2	B	355	GLU	2.2
2	B	299	THR	2.1
1	D	45	THR	2.1
2	B	342	ASN	2.1
2	B	275	ILE	2.1
1	D	285	THR	2.1
1	D	144	PRO	2.1
1	D	44	GLY	2.1
2	E	354	ALA	2.1
2	B	374	LEU	2.1
2	B	381	VAL	2.1
1	A	287	LEU	2.0
2	B	387	GLY	2.0
2	B	324	ARG	2.0
1	A	138	PRO	2.0
1	A	19	GLN	2.0
1	D	199	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

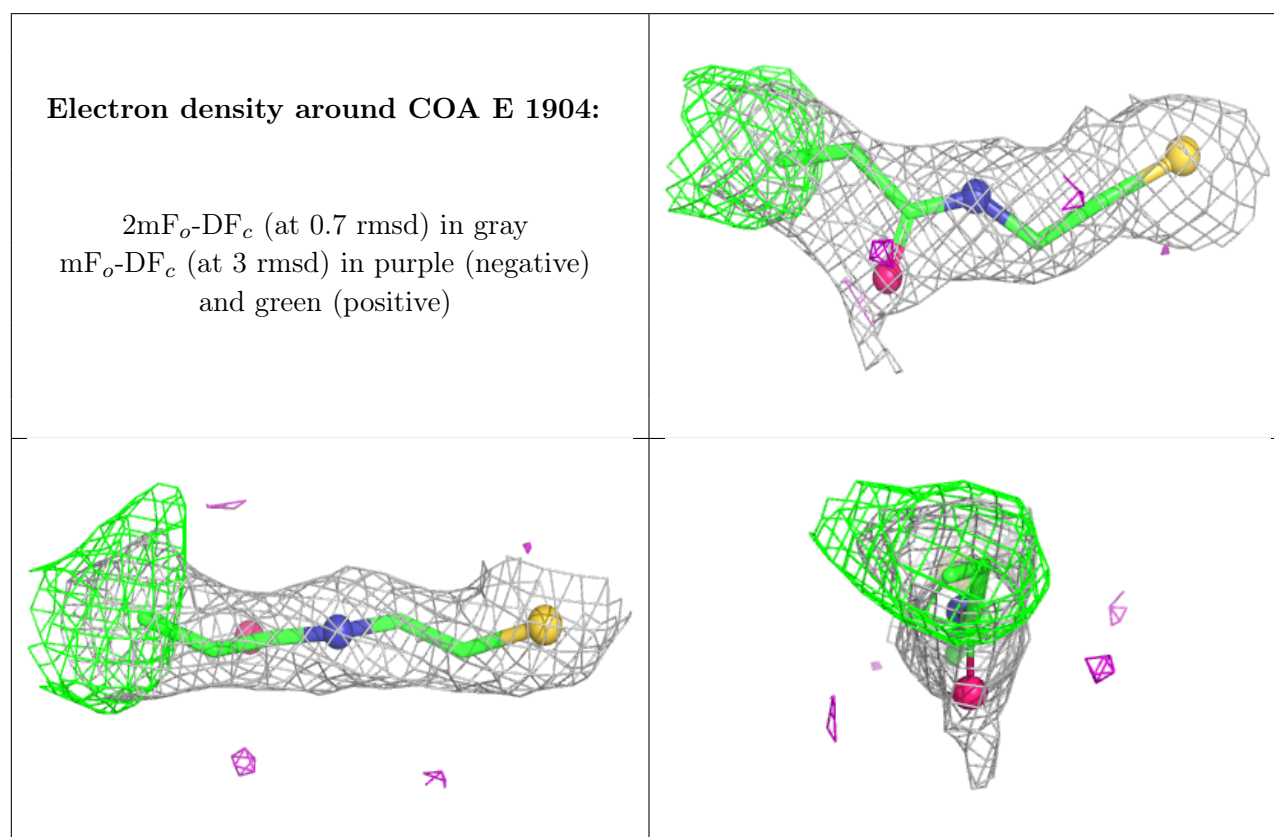
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	COA	E	1904	8/48	0.58	0.23	62,68,69,70	0
4	COA	B	1903	17/48	0.59	0.28	82,88,91,91	0
5	SO4	B	1500	5/5	0.86	0.23	34,34,36,37	5
4	COA	D	1301	42/48	0.92	0.10	50,61,67,68	0

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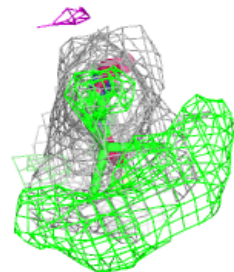
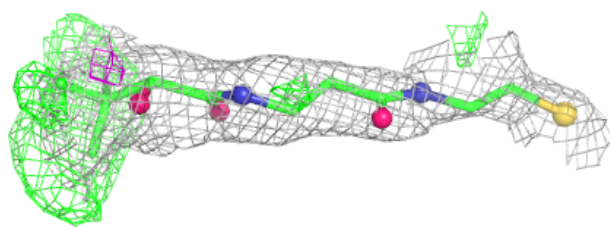
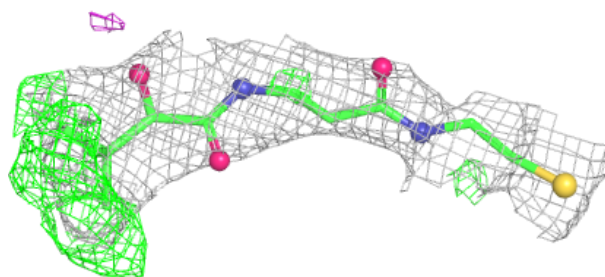
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	E	1501	5/5	0.92	0.10	70,71,71,71	0
5	SO4	E	1401	5/5	0.93	0.09	70,70,72,72	0
4	COA	A	1300	42/48	0.93	0.11	52,60,67,69	0
5	SO4	B	1400	5/5	0.94	0.10	59,60,61,63	0
3	PO4	A	1600	5/5	0.94	0.09	53,54,56,56	0
3	PO4	D	1601	5/5	0.97	0.06	54,57,57,58	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

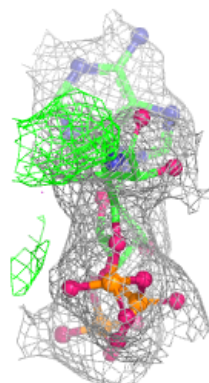
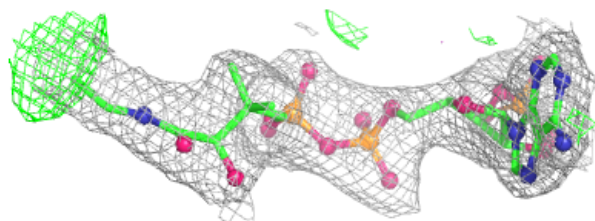
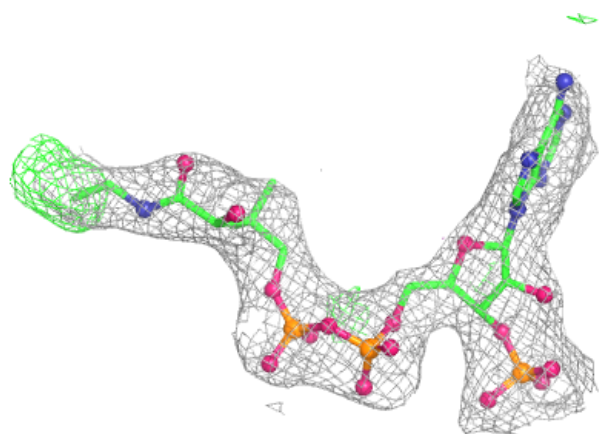


Electron density around COA B 1903:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

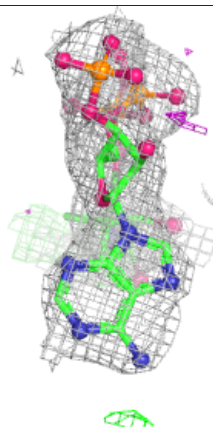
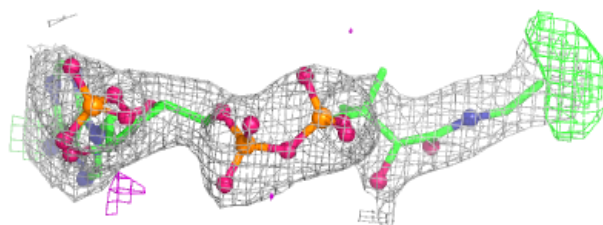
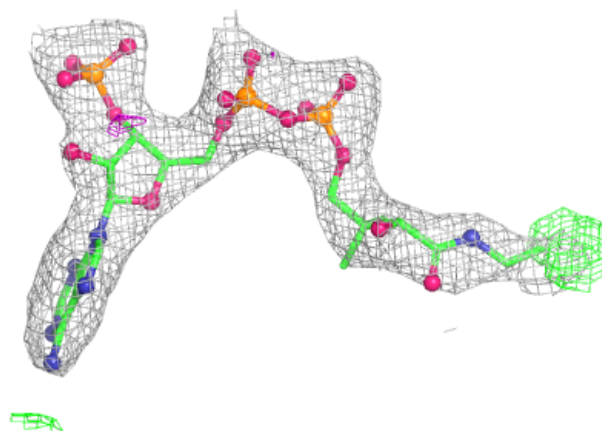
**Electron density around COA D 1301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around COA A 1300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.