



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:52 AM UTC

PDB ID : 4EAT / pdb_00004eat
Title : Crystal structure of a benzoate coenzyme A ligase
Authors : Geiger, J.; Strom, S.
Deposited on : 2012-03-22
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

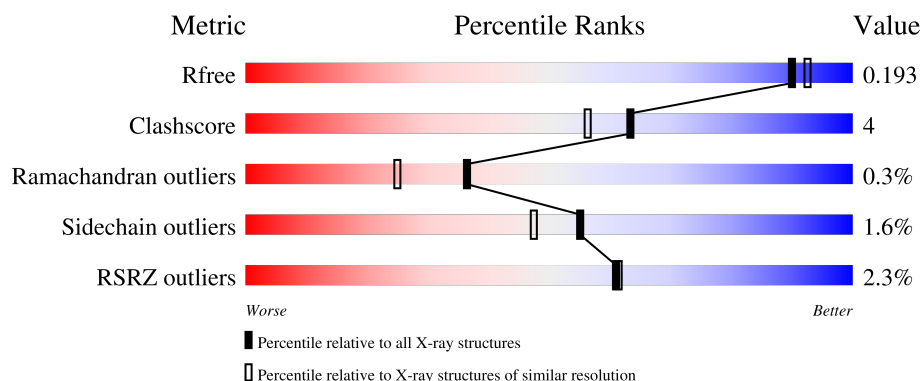
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	524	2% 86% 12% ..
1	B	524	2% 84% 13% ...

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BEZ	A	1000	-	X	-	-
2	BEZ	B	1000	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8566 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.

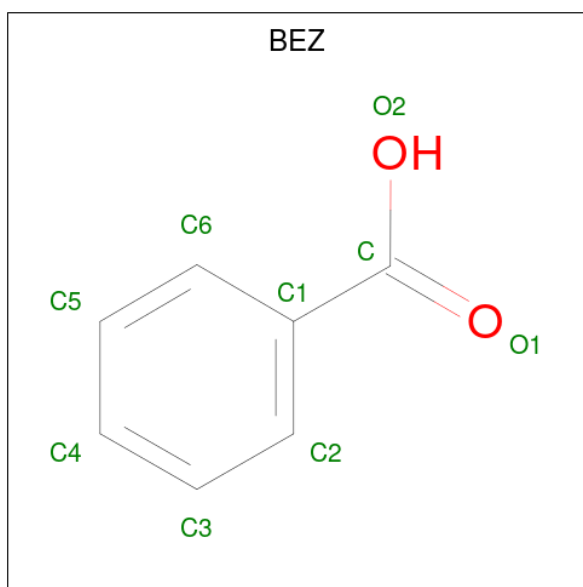
- Molecule 1 is a protein called Benzoate-coenzyme A ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	3	3	0
			3922	2514	678	721	9			
1	B	519	Total	C	N	O	S	12	5	0
			3944	2529	681	725	9			

There are 8 discrepancies between the modelled and reference sequences:

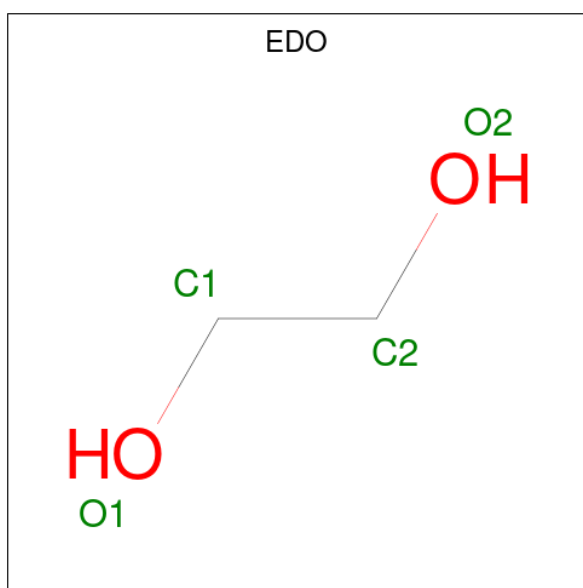
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q93TK0
A	83	ALA	THR	conflict	UNP Q93TK0
A	341	ASP	GLY	conflict	UNP Q93TK0
A	524	GLY	-	expression tag	UNP Q93TK0
B	1	MET	-	initiating methionine	UNP Q93TK0
B	83	ALA	THR	conflict	UNP Q93TK0
B	341	ASP	GLY	conflict	UNP Q93TK0
B	524	GLY	-	expression tag	UNP Q93TK0

- Molecule 2 is BENZOIC ACID (CCD ID: BEZ) (formula: C₇H₆O₂).



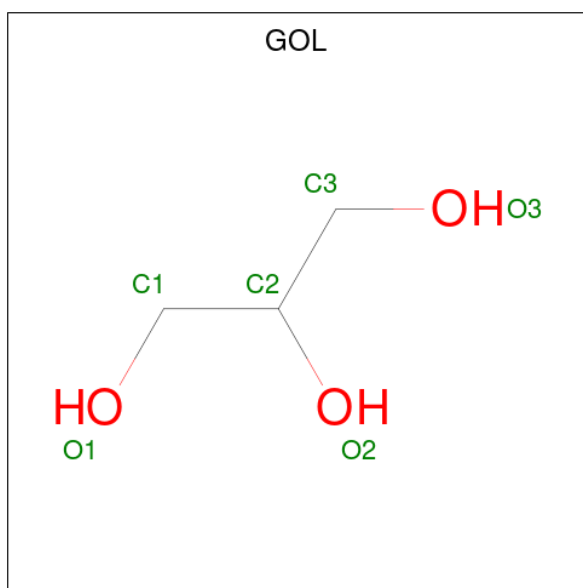
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	7	2		
2	B	1	Total	C	O	0	0
			9	7	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

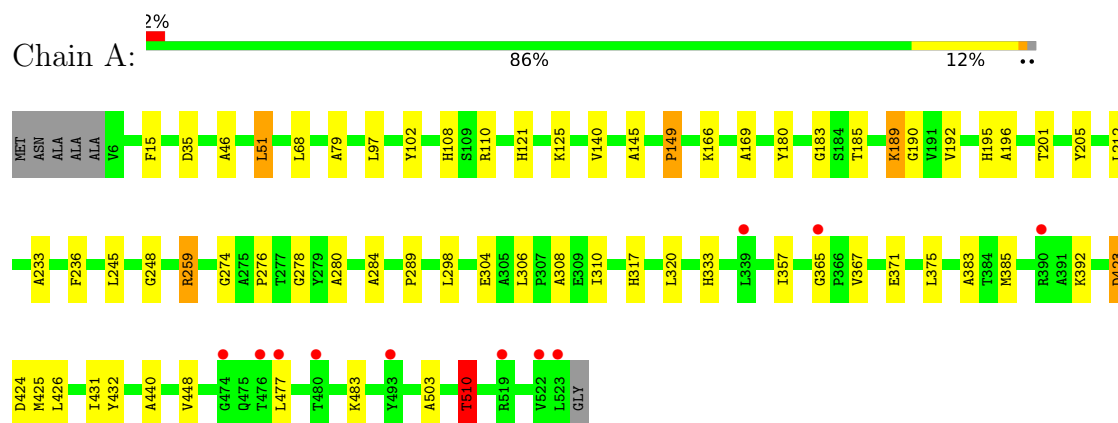
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	342	Total	O	0	0
			342	342		
5	B	314	Total	O	0	0
			314	314		

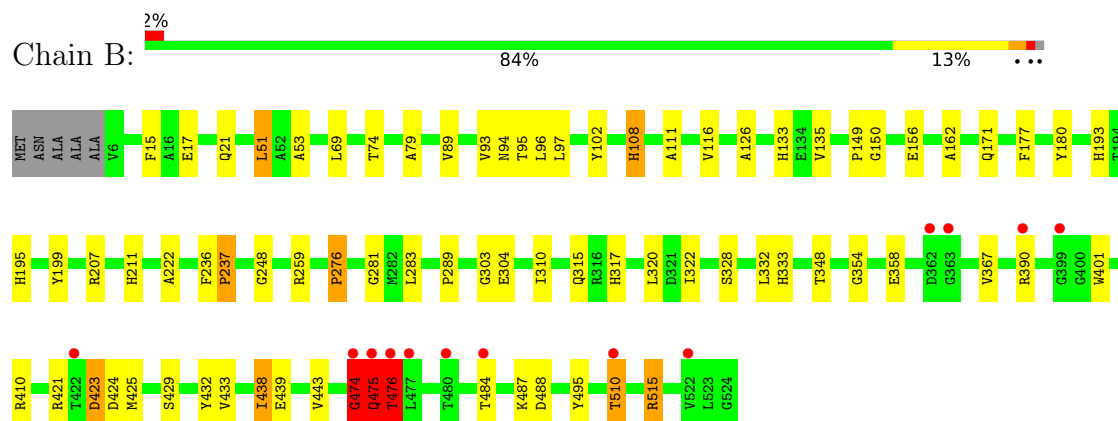
3 Residue-property plots

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: Benzoate-coenzyme A ligase



• Molecule 1: Benzoate-coenzyme A ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.65Å 96.02Å 95.38Å 90.00° 104.65° 90.00°	Depositor
Resolution (Å)	42.59 – 1.80 42.59 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (42.59-1.80) 98.6 (42.59-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.153 , 0.191 0.155 , 0.193	Depositor DCC
R_{free} test set	4702 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8566	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: GOL, EDO, BEZ

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	1.62	28/4035 (0.7%)	1.36	13/5506 (0.2%)
1	B	1.85	31/4064 (0.8%)	1.47	20/5544 (0.4%)
All	All	1.73	59/8099 (0.7%)	1.42	33/11050 (0.3%)

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	B	1	4

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	474	GLY	CA-C	-47.18	0.85	1.51
1	B	475	GLN	C-N	-24.69	0.99	1.33
1	B	476	THR	C-N	13.98	1.50	1.33
1	A	503	ALA	CA-CB	8.03	1.66	1.53
1	A	183	GLY	C-O	7.96	1.30	1.23
1	B	222	ALA	CA-CB	7.83	1.64	1.53
1	B	248	GLY	N-CA	7.25	1.54	1.45
1	A	367	VAL	CA-CB	7.22	1.64	1.54
1	A	196	ALA	CA-CB	7.17	1.65	1.53
1	A	140	VAL	CA-CB	6.94	1.62	1.53
1	A	233	ALA	CA-CB	6.54	1.63	1.53
1	A	185	THR	N-CA	6.20	1.54	1.45
1	B	310	ILE	CA-CB	6.18	1.61	1.54
1	B	108	HIS	CA-C	6.12	1.60	1.52
1	A	310	ILE	CA-CB	6.00	1.61	1.54
1	A	46	ALA	CA-CB	5.98	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	443	VAL	CA-CB	5.85	1.62	1.54
1	A	308	ALA	CA-CB	5.81	1.62	1.53
1	A	278	GLY	N-CA	5.79	1.52	1.45
1	A	284	ALA	N-CA	5.67	1.53	1.46
1	A	190	GLY	N-CA	5.62	1.53	1.45
1	A	192	VAL	CA-CB	5.61	1.60	1.54
1	B	111	ALA	N-CA	5.53	1.53	1.46
1	A	248	GLY	C-O	5.51	1.30	1.23
1	A	385	MET	C-O	5.50	1.29	1.23
1	B	367	VAL	CA-CB	5.50	1.63	1.55
1	B	53	ALA	N-CA	5.50	1.53	1.46
1	B	74	THR	CA-CB	5.49	1.62	1.53
1	A	274	GLY	N-CA	5.49	1.51	1.45
1	B	237	PRO	C-O	5.46	1.30	1.24
1	A	68	LEU	CA-C	5.44	1.59	1.53
1	A	306	LEU	CA-C	5.43	1.58	1.52
1	A	448	VAL	CA-CB	5.41	1.60	1.54
1	A	383	ALA	CA-CB	5.38	1.61	1.53
1	B	333	HIS	C-O	5.33	1.28	1.24
1	B	484	THR	CA-CB	5.32	1.61	1.53
1	B	93	VAL	N-CA	5.32	1.51	1.46
1	A	145	ALA	CA-CB	5.29	1.61	1.54
1	B	328	SER	N-CA	5.26	1.52	1.45
1	B	438	ILE	CA-CB	5.25	1.60	1.54
1	B	281	GLY	C-O	5.24	1.30	1.23
1	B	21	GLN	N-CA	5.24	1.52	1.46
1	B	135	VAL	N-CA	5.23	1.52	1.46
1	A	431	ILE	N-CA	5.21	1.52	1.46
1	B	475	GLN	CB-CG	5.21	1.68	1.52
1	B	354	GLY	N-CA	5.20	1.52	1.45
1	A	298	LEU	N-CA	5.19	1.52	1.46
1	B	495	TYR	CA-C	5.17	1.59	1.53
1	A	51	LEU	N-CA	5.13	1.52	1.46
1	B	439	GLU	CB-CG	-5.13	1.37	1.52
1	A	333	HIS	N-CA	5.11	1.52	1.46
1	B	322	ILE	C-O	5.10	1.30	1.24
1	B	515	ARG	CA-C	5.04	1.59	1.52
1	B	156[A]	GLU	C-O	5.03	1.29	1.24
1	B	156[B]	GLU	C-O	5.03	1.29	1.24
1	B	17	GLU	N-CA	5.03	1.52	1.46
1	A	169	ALA	CA-CB	5.02	1.59	1.52
1	B	199	TYR	C-O	5.01	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	ALA	N-CA	5.00	1.52	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	475	GLN	O-C-N	-39.21	70.44	122.59
1	B	476	THR	O-C-N	-15.86	101.50	122.59
1	B	475	GLN	CB-CG-CD	-15.58	86.11	112.60
1	B	476	THR	CB-CA-C	-13.11	84.32	110.42
1	B	476	THR	N-CA-C	13.04	138.58	110.80
1	B	474	GLY	N-CA-C	12.94	143.84	113.18
1	A	365	GLY	CA-C-N	9.59	129.68	119.90
1	A	365	GLY	C-N-CA	9.59	129.68	119.90
1	B	475	GLN	CB-CA-C	7.65	125.64	110.42
1	A	423	ASP	N-CA-C	7.29	119.72	110.61
1	A	110	ARG	CG-CD-NE	-6.65	97.36	112.00
1	B	439	GLU	CB-CA-C	-6.48	100.70	110.88
1	B	475	GLN	CA-C-N	6.30	133.58	121.54
1	B	475	GLN	C-N-CA	6.30	133.58	121.54
1	A	259	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	A	166	LYS	CA-C-N	-5.92	114.66	120.52
1	A	166	LYS	C-N-CA	-5.92	114.66	120.52
1	B	162	ALA	CA-C-N	-5.73	113.86	119.76
1	B	162	ALA	C-N-CA	-5.73	113.86	119.76
1	B	303	GLY	N-CA-C	-5.72	107.67	114.48
1	B	150	GLY	N-CA-C	-5.69	106.86	114.25
1	A	510	THR	N-CA-CB	-5.60	102.19	110.53
1	B	348	THR	N-CA-C	-5.53	106.41	112.72
1	A	201	THR	N-CA-C	-5.38	105.58	111.82
1	A	423	ASP	CB-CA-C	-5.31	102.22	111.35
1	B	423	ASP	CA-C-N	-5.31	117.08	126.32
1	B	423	ASP	C-N-CA	-5.31	117.08	126.32
1	A	483	LYS	N-CA-C	5.23	116.67	111.07
1	A	205	TYR	CA-C-N	-5.17	114.24	119.98
1	A	205	TYR	C-N-CA	-5.17	114.24	119.98
1	B	133	HIS	N-CA-C	-5.17	102.81	110.46
1	B	259	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	B	94	ASN	N-CA-CB	-5.02	102.25	109.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	476	THR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	474	GLY	Mainchain
1	B	475	GLN	Mainchain,Peptide
1	B	476	THR	Peptide

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	3922	0	3843	29	0
1	B	3944	0	3875	42	0
2	A	9	0	5	0	0
2	B	9	0	5	0	0
3	A	4	0	6	0	0
3	B	4	0	6	1	0
4	B	18	0	24	3	0
5	A	342	0	0	4	0
5	B	314	0	0	5	0
All	All	8566	0	7764	62	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 4.

All (62) 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:510:THR:HG23	1:B:149:PRO:HG3	1.41	1.00
1:B:423:ASP:O	1:B:424:ASP:HB2	1.66	0.93
1:B:95:THR:OG1	4:B:1002:GOL:H12	1.72	0.90
1:A:15:PHE:H	1:A:195:HIS:HD2	1.18	0.89
1:B:15:PHE:H	1:B:195:HIS:HD2	1.20	0.86
1:A:510:THR:HG23	1:B:149:PRO:CG	2.04	0.86
1:A:510:THR:CG2	1:B:149:PRO:CG	2.60	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASP:CB	5:A:1344:HOH:O	2.31	0.77
1:A:149:PRO:CG	1:B:510:THR:HG23	2.16	0.76
1:A:35:ASP:OD2	5:A:1189:HOH:O	2.05	0.73
1:A:510:THR:CG2	1:B:149:PRO:HG2	2.18	0.73
1:A:15:PHE:H	1:A:195:HIS:CD2	2.07	0.72
1:B:488:ASP:CB	5:B:1383:HOH:O	2.37	0.71
1:B:488:ASP:CB	5:B:1273:HOH:O	2.38	0.70
1:A:189:LYS:HD3	1:A:392:LYS:HD3	1.73	0.69
1:B:421:ARG:HH21	1:B:423:ASP:CG	2.03	0.66
1:A:149:PRO:HG2	1:B:510:THR:HG23	1.78	0.64
1:B:108:HIS:HD2	1:B:180:TYR:OH	1.80	0.64
1:A:108:HIS:HD2	1:A:180:TYR:OH	1.81	0.62
1:B:96:LEU:HG	4:B:1002:GOL:H11	1.82	0.62
1:B:515:ARG:HD3	5:B:1302:HOH:O	2.00	0.61
1:A:195:HIS:HE1	5:A:1269:HOH:O	1.86	0.57
1:B:289:PRO:O	1:B:317:HIS:HE1	1.88	0.57
1:A:510:THR:HG21	1:B:149:PRO:HG2	1.85	0.57
1:A:245:LEU:HD21	1:A:259:ARG:HG2	1.86	0.57
1:A:289:PRO:O	1:A:317:HIS:HE1	1.88	0.56
1:B:15:PHE:H	1:B:195:HIS:CD2	2.12	0.56
1:B:358:GLU:HG3	1:B:401:TRP:CH2	2.41	0.56
1:A:149:PRO:HG2	1:B:510:THR:CG2	2.37	0.54
1:A:121:HIS:CE1	1:A:125:LYS:HE3	2.43	0.53
1:B:195:HIS:HE1	5:B:1187:HOH:O	1.92	0.52
1:B:410:ARG:CZ	3:B:1004:EDO:H12	2.40	0.51
1:B:515:ARG:HH21	1:B:515:ARG:HG3	1.74	0.51
1:B:515:ARG:HG3	1:B:515:ARG:NH2	2.27	0.49
1:B:421:ARG:NH2	1:B:423:ASP:OD2	2.38	0.48
1:A:51:LEU:CD2	1:A:79:ALA:HA	2.45	0.47
1:B:207:ARG:O	1:B:211:HIS:HA	2.15	0.46
1:B:193:HIS:CE1	1:B:332:LEU:HB2	2.51	0.46
1:B:89:VAL:HG13	1:B:177:PHE:HA	1.97	0.46
1:B:97:LEU:HB2	1:B:102:TYR:CZ	2.52	0.45
1:A:276:PRO:HD2	1:A:304:GLU:HG2	1.99	0.45
1:A:425:MET:CE	1:A:432:TYR:HB3	2.47	0.45
1:A:357:ILE:HG23	1:A:375:LEU:HD11	1.97	0.45
1:A:423:ASP:OD1	1:A:423:ASP:C	2.58	0.43
1:B:276:PRO:HD2	1:B:304:GLU:HG2	2.00	0.43
1:B:51[B]:LEU:HD23	1:B:79:ALA:HA	2.01	0.43
1:B:96:LEU:HD11	4:B:1002:GOL:H31	2.01	0.43
1:A:425:MET:HE3	1:A:432:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:MET:HB3	1:B:432:TYR:HD1	1.84	0.42
1:A:212:LEU:HD12	1:A:236:PHE:HB3	2.01	0.42
1:A:97:LEU:HB2	1:A:102:TYR:CZ	2.54	0.42
1:B:283:LEU:HD23	1:B:283:LEU:HA	1.89	0.42
1:B:315:GLN:HA	1:B:320:LEU:O	2.20	0.41
1:B:433:VAL:HG11	1:B:438:ILE:HD11	2.02	0.41
1:B:487:LYS:HB2	1:B:487:LYS:HE3	1.70	0.41
1:B:236:PHE:HB2	1:B:237:PRO:CD	2.50	0.41
1:A:371:GLU:HG2	5:A:1387:HOH:O	2.19	0.41
1:A:440:ALA:HB1	1:B:126:ALA:HA	2.03	0.41
1:B:488:ASP:CA	5:B:1273:HOH:O	2.67	0.41
1:B:51[B]:LEU:CD2	1:B:79:ALA:HA	2.51	0.41
1:A:245:LEU:HD21	1:A:259:ARG:CG	2.51	0.41
1:B:69:LEU:O	1:B:116:VAL:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	519/524 (99%)	505 (97%)	14 (3%)	0	100	100
1	B	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	21	11
All	All	1041/1048 (99%)	1013 (97%)	25 (2%)	3 (0%)	36	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	474	GLY
1	B	475	GLN
1	B	476	THR

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	397/414 (96%)	391 (98%)	6 (2%)	57	49
1	B	401/414 (97%)	392 (98%)	9 (2%)	45	34
All	All	798/828 (96%)	783 (98%)	15 (2%)	55	41

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	PRO
1	A	189	LYS
1	A	320	LEU
1	A	426	LEU
1	A	477	LEU
1	A	510	THR
1	B	51[A]	LEU
1	B	51[B]	LEU
1	B	171	GLN
1	B	276	PRO
1	B	390	ARG
1	B	429[A]	SER
1	B	429[B]	SER
1	B	475	GLN
1	B	510	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	136	GLN
1	A	195	HIS
1	A	317	HIS
1	A	378	HIS
1	A	460	HIS
1	A	514	GLN

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Mol	Chain	Res	Type
1	B	108	HIS
1	B	161	HIS
1	B	195	HIS
1	B	317	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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$
2	BEZ	A	1000	-	9,9,9	0.98	0	11,11,11	2.20	7 (63%)
2	BEZ	B	1000	-	9,9,9	2.08	2 (22%)	11,11,11	2.65	8 (72%)
4	GOL	B	1003	-	5,5,5	0.47	0	5,5,5	0.84	0
3	EDO	B	1004	-	3,3,3	0.79	0	2,2,2	0.03	0
4	GOL	B	1001	-	5,5,5	1.08	0	5,5,5	1.35	1 (20%)
3	EDO	A	1001	-	3,3,3	0.67	0	2,2,2	0.65	0
4	GOL	B	1002	-	5,5,5	0.79	0	5,5,5	2.74	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BEZ	A	1000	-	-	4/4/4/4	0/1/1/1
2	BEZ	B	1000	-	-	4/4/4/4	0/1/1/1
4	GOL	B	1003	-	-	1/4/4/4	-
3	EDO	B	1004	-	-	1/1/1/1	-
4	GOL	B	1001	-	-	0/4/4/4	-
3	EDO	A	1001	-	-	1/1/1/1	-
4	GOL	B	1002	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	BEZ	C5-C6	4.19	1.46	1.38
2	B	1000	BEZ	C5-C4	2.45	1.43	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	BEZ	C6-C1-C2	5.04	124.98	118.57
4	B	1002	GOL	O1-C1-C2	4.19	129.26	110.38
4	B	1002	GOL	O2-C2-C1	3.86	125.14	109.18
2	A	1000	BEZ	C6-C1-C2	3.49	123.00	118.57
2	B	1000	BEZ	C5-C6-C1	-3.38	117.04	120.36
2	B	1000	BEZ	C2-C1-C	-3.13	114.19	120.37
2	A	1000	BEZ	C6-C1-C	-3.11	114.21	120.37
4	B	1001	GOL	O2-C2-C1	-2.81	97.55	109.18
2	B	1000	BEZ	C3-C2-C1	-2.68	117.73	120.36
2	B	1000	BEZ	C5-C4-C3	2.65	123.50	119.87
2	A	1000	BEZ	C4-C5-C6	-2.60	117.03	120.24
2	A	1000	BEZ	C5-C4-C3	2.59	123.41	119.87
2	B	1000	BEZ	O2-C-C1	2.44	121.11	114.84
2	A	1000	BEZ	O2-C-C1	2.22	120.55	114.84
2	B	1000	BEZ	O2-C-O1	-2.17	118.69	123.35
2	A	1000	BEZ	C3-C2-C1	-2.15	118.26	120.36
2	B	1000	BEZ	C4-C5-C6	-2.10	117.65	120.24
2	A	1000	BEZ	O2-C-O1	-2.05	118.95	123.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1002	GOL	O1-C1-C2-C3
2	A	1000	BEZ	O2-C-C1-C6
2	A	1000	BEZ	O1-C-C1-C6
2	B	1000	BEZ	O1-C-C1-C6
2	A	1000	BEZ	O2-C-C1-C2
2	B	1000	BEZ	O1-C-C1-C2
4	B	1002	GOL	O1-C1-C2-O2
4	B	1003	GOL	C1-C2-C3-O3
2	A	1000	BEZ	O1-C-C1-C2
4	B	1002	GOL	O2-C2-C3-O3
2	B	1000	BEZ	O2-C-C1-C6
2	B	1000	BEZ	O2-C-C1-C2
3	A	1001	EDO	O1-C1-C2-O2
3	B	1004	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1004	EDO	1	0
4	B	1002	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	475:GLN	C	476:THR	N	0.99

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	518/524 (98%)	-0.39	11 (2%) 63 64	6, 17, 34, 55	7 (1%)
1	B	519/524 (99%)	-0.30	13 (2%) 58 58	5, 18, 34, 44	9 (1%)
All	All	1037/1048 (98%)	-0.34	24 (2%) 61 61	5, 17, 34, 55	16 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	475	GLN	15.4
1	B	476	THR	8.9
1	A	523	LEU	6.0
1	B	474	GLY	5.8
1	A	476	THR	4.8
1	A	522	VAL	4.7
1	A	519	ARG	4.0
1	B	362	ASP	2.9
1	B	399	GLY	2.7
1	A	493	TYR	2.7
1	A	390	ARG	2.5
1	A	339	LEU	2.4
1	B	522	VAL	2.4
1	B	477	LEU	2.3
1	B	422	THR	2.3
1	B	480	THR	2.3
1	A	480	THR	2.2
1	B	510	THR	2.2
1	B	484	THR	2.2
1	A	477	LEU	2.1
1	A	365	GLY	2.1
1	B	390	ARG	2.1
1	A	474	GLY	2.0
1	B	363	GLY	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	GOL	B	1002	6/6	0.85	0.12	18,32,37,38	0
3	EDO	B	1004	4/4	0.86	0.11	28,35,38,39	0
3	EDO	A	1001	4/4	0.92	0.08	20,25,33,33	0
4	GOL	B	1003	6/6	0.92	0.09	22,34,39,39	0
4	GOL	B	1001	6/6	0.94	0.10	20,21,24,26	0
2	BEZ	A	1000	9/9	0.96	0.06	12,15,17,18	0
2	BEZ	B	1000	9/9	0.98	0.06	10,14,16,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.