Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 12:38 PM EST

PDB ID	:	4EAT
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 (i) 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 (1)) were used in the production of this report:

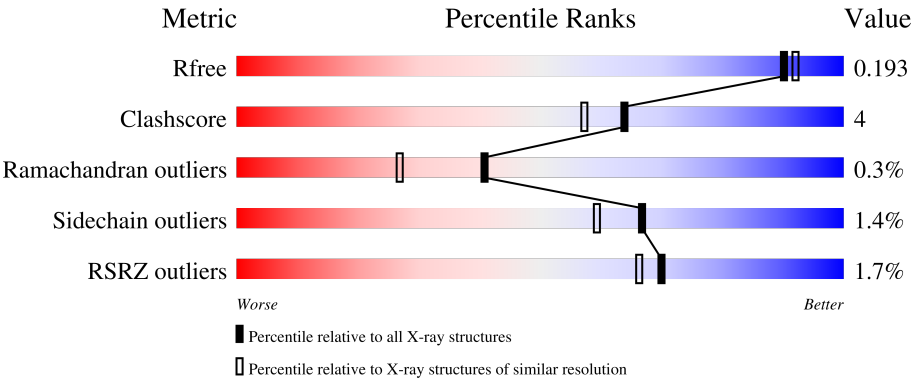
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 <=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% 89% 9%
1	B	524	% 85% 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	B	1000	-	X	-	-
4	GOL	B	1002	-	X	-	-

2 Entry composition (i)

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.

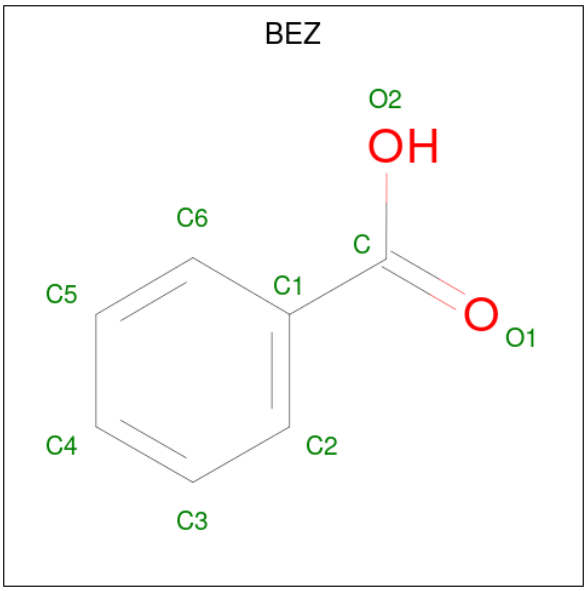
- Molecule 1 is a protein called Benzoate-coenzyme A ligase.

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:

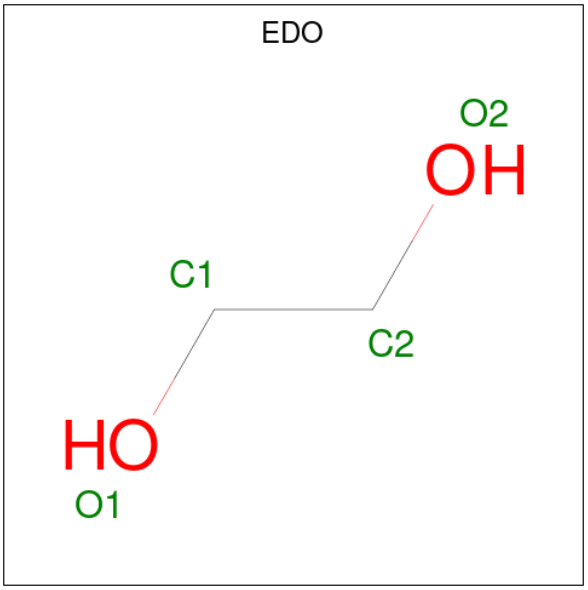
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q93TK0
A	83	ALA	THR	conflict	UNP Q93TK0
A	341	ASP	GLY	conflict	UNP Q93TK0
A	524	GLY	-	expression tag	UNP Q93TK0
B	1	MET	-	initiating methionine	UNP Q93TK0
B	83	ALA	THR	conflict	UNP Q93TK0
B	341	ASP	GLY	conflict	UNP Q93TK0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

- Molecule 2 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



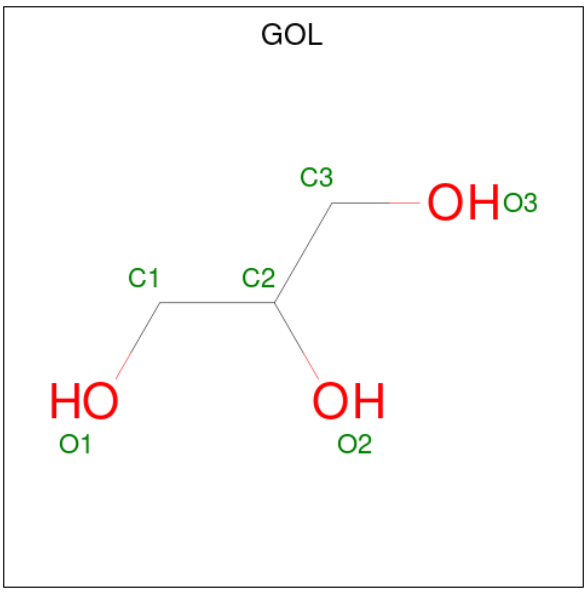
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 7 2	0	0
2	B	1	Total C O 9 7 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

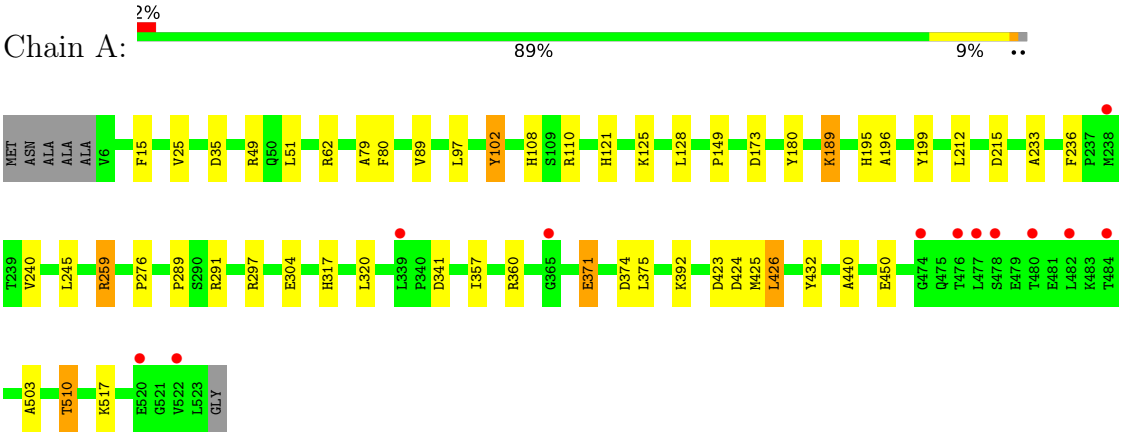
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	342	Total O 342 342	0	0
5	B	314	Total O 314 314	0	0

3 Residue-property plots (i)

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.

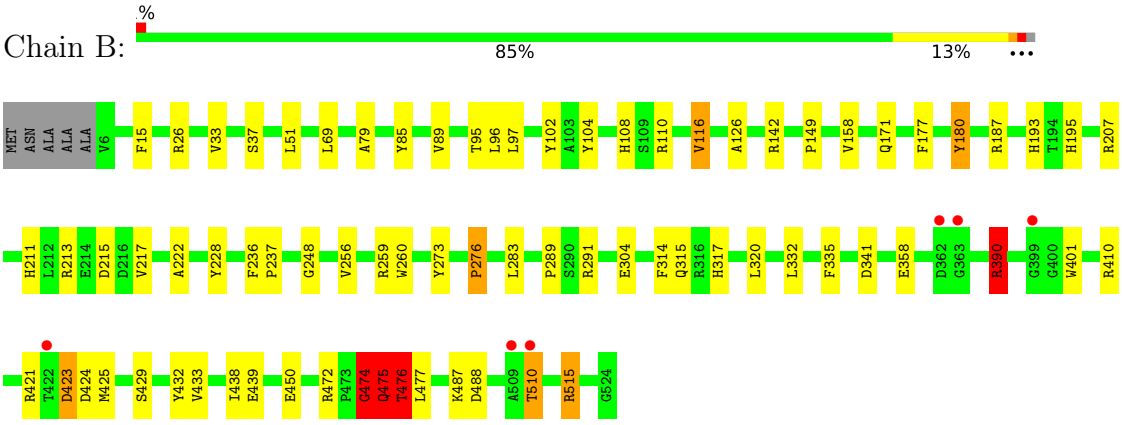
• Molecule 1: Benzoate-coenzyme A ligase

Chain A:



• Molecule 1: Benzoate-coenzyme A ligase

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.02%)	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)	0.39 , 53.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, BEZ, EDO

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	1.38	11/4035 (0.3%)	1.14	16/5506 (0.3%)
1	B	1.56	25/4064 (0.6%)	1.30	25/5544 (0.5%)
All	All	1.47	36/8099 (0.4%)	1.23	41/11050 (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	B	1	4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	474	GLY	CA-C	-41.56	0.85	1.51
1	B	475	GLN	C-N	-15.18	0.99	1.34
1	B	439	GLU	CB-CG	-7.94	1.37	1.52
1	B	476	THR	C-N	7.26	1.50	1.34
1	A	199	TYR	CD2-CE2	6.72	1.49	1.39
1	A	503	ALA	CA-CB	6.67	1.66	1.52
1	A	240	VAL	CB-CG2	6.31	1.66	1.52
1	A	196	ALA	CA-CB	6.07	1.65	1.52
1	B	110	ARG	CG-CD	5.91	1.66	1.51
1	B	228	TYR	CE1-CZ	5.87	1.46	1.38
1	B	104	TYR	CE2-CZ	5.84	1.46	1.38
1	B	217	VAL	CB-CG2	5.83	1.65	1.52
1	B	248	GLY	N-CA	5.76	1.54	1.46
1	B	256	VAL	CB-CG1	5.75	1.65	1.52
1	B	475	GLN	CB-CG	5.75	1.68	1.52
1	B	260	TRP	CZ3-CH2	5.71	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	PHE	CD2-CE2	5.67	1.50	1.39
1	A	25	VAL	CB-CG1	5.64	1.64	1.52
1	A	371	GLU	CG-CD	5.62	1.60	1.51
1	A	259	ARG	CG-CD	-5.60	1.38	1.51
1	B	222	ALA	CA-CB	5.49	1.64	1.52
1	B	450	GLU	CB-CG	-5.48	1.41	1.52
1	B	273	TYR	CE2-CZ	5.45	1.45	1.38
1	A	450	GLU	CB-CG	-5.40	1.41	1.52
1	B	116	VAL	CB-CG1	5.31	1.64	1.52
1	B	180	TYR	CD1-CE1	5.31	1.47	1.39
1	B	314	PHE	CE1-CZ	5.28	1.47	1.37
1	B	158	VAL	CB-CG1	5.27	1.64	1.52
1	B	33	VAL	CB-CG2	5.24	1.63	1.52
1	B	37	SER	CB-OG	5.22	1.49	1.42
1	B	259	ARG	CG-CD	-5.22	1.38	1.51
1	A	80	PHE	CD1-CE1	5.22	1.49	1.39
1	A	233	ALA	CA-CB	5.21	1.63	1.52
1	A	102	TYR	CG-CD2	5.15	1.45	1.39
1	B	26	ARG	CG-CD	5.09	1.64	1.51
1	B	85	TYR	CD1-CE1	5.06	1.47	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	475	GLN	O-C-N	-32.66	70.44	122.70
1	B	475	GLN	CA-C-N	21.31	164.07	117.20
1	B	476	THR	O-C-N	-13.25	101.50	122.70
1	B	474	GLY	N-CA-C	12.30	143.84	113.10
1	B	476	THR	CA-C-N	12.12	143.87	117.20
1	B	476	THR	N-CA-C	10.22	138.58	111.00
1	B	476	THR	CB-CA-C	-10.10	84.32	111.60
1	B	475	GLN	CB-CG-CD	-9.80	86.11	111.60
1	A	259	ARG	NE-CZ-NH1	-9.67	115.46	120.30
1	B	515	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	B	291	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	B	291	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	B	215	ASP	CB-CG-OD1	7.92	125.42	118.30
1	B	475	GLN	CB-CA-C	7.62	125.64	110.40
1	B	341	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	173	ASP	CB-CG-OD2	7.02	124.62	118.30
1	A	110	ARG	CG-CD-NE	-6.88	97.36	111.80
1	B	341	ASP	CB-CG-OD1	6.71	124.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	341	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	426	LEU	CB-CG-CD1	6.67	122.35	111.00
1	B	515	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	477	LEU	CA-CB-CG	6.50	130.25	115.30
1	A	215	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	213	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	291	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	297	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	215	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	B	390	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	A	49	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	360	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	B	187	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	142	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	374	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	62	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	B	423	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	128	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	B	228	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	517	LYS	CD-CE-NZ	-5.22	99.70	111.70
1	B	110	ARG	CD-NE-CZ	5.20	130.88	123.60
1	A	291	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	89	VAL	CG1-CB-CG2	-5.02	102.86	110.90

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	Peptide,Mainchain
1	B	476	THR	Peptide

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3922	0	3843	28	0
1	B	3944	0	3875	47	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	66	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 (66) 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:B:390:ARG:HH11	1:B:390:ARG:CG	1.36	1.32
1:B:390:ARG:HG3	1:B:390:ARG:NH1	1.49	1.04
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:390:ARG:HH11	1:B:390:ARG:HG3	0.79	0.93
1:B:390:ARG:CG	1:B:390:ARG:NH1	2.13	0.91
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
1:A:424:ASP:CB	5:A:1344:HOH:O	2.31	0.77
1:B:390:ARG:HH11	1:B:390:ARG:HG2	1.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LEU:HG	4:B:1002:GOL:H11	1.82	0.62
1:B:421:ARG:HH21	1:B:423:ASP:CG	2.03	0.61
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ASP:C	1:A:423:ASP:OD1	2.58	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%)	25 12
All	All	1041/1048 (99%)	1013 (97%)	25 (2%)	3 (0%)	41 27

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	397/414 (96%)	393 (99%)	4 (1%)	76 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	401/414 (97%)	393 (98%)	8 (2%)	55 44
All	All	798/828 (96%)	786 (98%)	12 (2%)	67 56

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	LYS
1	A	320	LEU
1	A	426	LEU
1	A	510	THR
1	B	171	GLN
1	B	276	PRO
1	B	390	ARG
1	B	429[A]	SER
1	B	429[B]	SER
1	B	472	ARG
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	50	GLN
1	A	108	HIS
1	A	112	GLN
1	A	136	GLN
1	A	195	HIS
1	A	317	HIS
1	B	50	GLN
1	B	108	HIS
1	B	112	GLN
1	B	195	HIS
1	B	317	HIS

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 monosaccharides 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	$\#\|Z\| > 2$
4	GOL	B	1003	-	5,5,5	0.45	0	5,5,5	0.78	0
3	EDO	A	1001	-	3,3,3	0.68	0	2,2,2	0.64	0
2	BEZ	A	1000	-	9,9,9	0.90	0	11,11,11	1.96	4 (36%)
4	GOL	B	1001	-	5,5,5	1.03	0	5,5,5	1.27	1 (20%)
4	GOL	B	1002	-	5,5,5	0.76	0	5,5,5	2.59	2 (40%)
3	EDO	B	1004	-	3,3,3	0.83	0	2,2,2	0.07	0
2	BEZ	B	1000	-	9,9,9	1.79	2 (22%)	11,11,11	2.34	6 (54%)

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	GOL	B	1003	-	-	1/4/4/4	-
3	EDO	A	1001	-	-	1/1/1/1	-
2	BEZ	A	1000	-	-	4/4/4/4	0/1/1/1
4	GOL	B	1001	-	-	0/4/4/4	-
4	GOL	B	1002	-	-	4/4/4/4	-
3	EDO	B	1004	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BEZ	B	1000	-	-	4/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	BEZ	C5-C6	3.40	1.46	1.38
2	B	1000	BEZ	C5-C4	2.12	1.43	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1000	BEZ	C6-C1-C2	4.49	124.98	118.59
4	B	1002	GOL	O1-C1-C2	3.97	129.26	110.20
4	B	1002	GOL	O2-C2-C1	3.64	125.14	109.12
2	B	1000	BEZ	C2-C1-C	-3.15	114.19	120.39
2	A	1000	BEZ	C6-C1-C	-3.14	114.21	120.39
2	A	1000	BEZ	C6-C1-C2	3.10	123.00	118.59
2	B	1000	BEZ	C5-C6-C1	-2.79	117.04	120.34
4	B	1001	GOL	O2-C2-C1	-2.63	97.55	109.12
2	B	1000	BEZ	O2-C-C1	2.41	121.11	114.85
2	B	1000	BEZ	C3-C2-C1	-2.20	117.73	120.34
2	A	1000	BEZ	O2-C-C1	2.20	120.55	114.85
2	B	1000	BEZ	O2-C-O1	-2.10	118.69	123.35
2	A	1000	BEZ	C4-C5-C6	-2.08	117.03	120.19

There are no chirality outliers.

All (15) 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
2	A	1000	BEZ	O1-C-C1-C2
2	B	1000	BEZ	O2-C-C1-C6
4	B	1003	GOL	C1-C2-C3-O3
2	B	1000	BEZ	O2-C-C1-C2
4	B	1002	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	1001	EDO	O1-C1-C2-O2
3	B	1004	EDO	O1-C1-C2-O2
4	B	1002	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1002	GOL	3	0
3	B	1004	EDO	1	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, 95^{th} 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%)	-0.31	12 (2%) 60 56	8, 17, 34, 55	5 (0%)
1	B	519/524 (99%)	-0.34	6 (1%) 79 76	9, 18, 34, 52	4 (0%)
All	All	1037/1048 (98%)	-0.33	18 (1%) 70 66	8, 17, 34, 55	9 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	THR	5.9
1	A	484	THR	3.9
1	B	362	ASP	3.8
1	A	474	GLY	3.7
1	B	399	GLY	3.7
1	A	339	LEU	3.2
1	B	510	THR	3.2
1	A	522	VAL	3.1
1	B	509	ALA	2.9
1	A	478	SER	2.8
1	B	363	GLY	2.8
1	A	477	LEU	2.7
1	A	482	LEU	2.7
1	A	365	GLY	2.5
1	A	520	GLU	2.4
1	B	422	THR	2.3
1	A	238	MET	2.1
1	A	480	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
4	GOL	B	1002	6/6	0.88	0.11	18,32,37,38	0
3	EDO	B	1004	4/4	0.92	0.17	28,35,38,39	0
4	GOL	B	1003	6/6	0.94	0.19	22,34,39,39	0
4	GOL	B	1001	6/6	0.96	0.07	20,21,24,26	0
2	BEZ	A	1000	9/9	0.97	0.10	12,15,17,18	0
2	BEZ	B	1000	9/9	0.97	0.06	10,14,16,17	0
3	EDO	A	1001	4/4	0.98	0.07	20,25,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.