wwPDB X-ray Structure Validation Summary Report (i)

Dec 12, 2023 – 05:48 pm GMT

PDB ID	:	3ZDS
Title	:	Structure of homogentisate 1,2-dioxygenase in complex with reaction intermediates of homogentisate with oxygen.
Authors	:	Jeoung, J.-H.; Bommer, M.; Lin, T.-Y.; Dobbek, H.
Deposited on	:	2012-11-30
Resolution	:	1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

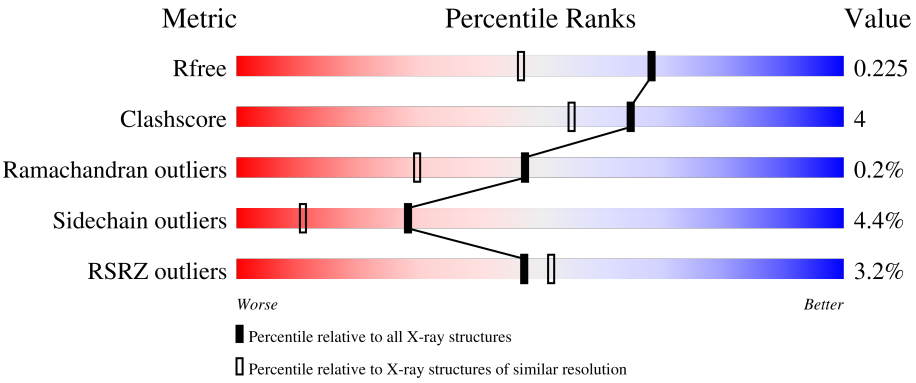
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	433	2% 88% 10% ·
1	B	433	2% 91% 7% ·
1	C	433	3% 89% 9% ·
1	D	433	2% 85% 12% ·
1	E	433	3% 86% 11% ··

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Mol	Chain	Length	Quality of chain
1	F	433	3% 87% 10%
1	G	433	3% 88% 9%
1	H	433	4% 84% 13%
1	I	433	3% 84% 13%
1	J	433	2% 88% 9%
1	K	433	7% 83% 14%
1	L	433	4% 85% 12%

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	M8O	A	2001	-	X	-	-
5	OXY	C	1999	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 46082 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 HOMOGENTISATE 1,2-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	16	5	0
			3365	2149	595	604	17			
1	B	426	Total	C	N	O	S	7	4	0
			3358	2145	590	606	17			
1	C	426	Total	C	N	O	S	12	3	0
			3350	2138	590	605	17			
1	D	426	Total	C	N	O	S	9	6	0
			3372	2154	596	605	17			
1	E	426	Total	C	N	O	S	5	3	0
			3351	2139	591	604	17			
1	F	426	Total	C	N	O	S	5	5	0
			3366	2151	595	603	17			
1	G	425	Total	C	N	O	S	5	3	0
			3339	2133	587	601	18			
1	H	426	Total	C	N	O	S	1	2	0
			3343	2134	588	604	17			
1	I	426	Total	C	N	O	S	8	1	0
			3335	2129	585	604	17			
1	J	426	Total	C	N	O	S	4	3	0
			3350	2141	588	603	18			
1	K	426	Total	C	N	O	S	4	3	0
			3351	2140	589	604	18			
1	L	426	Total	C	N	O	S	1	0	0
			3332	2127	585	603	17			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

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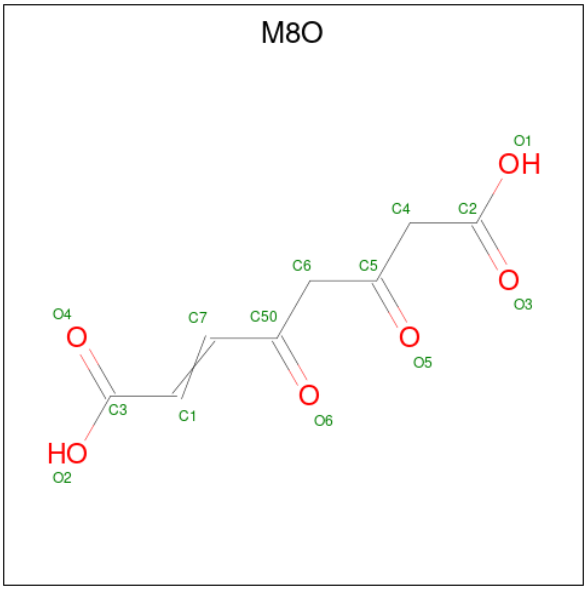
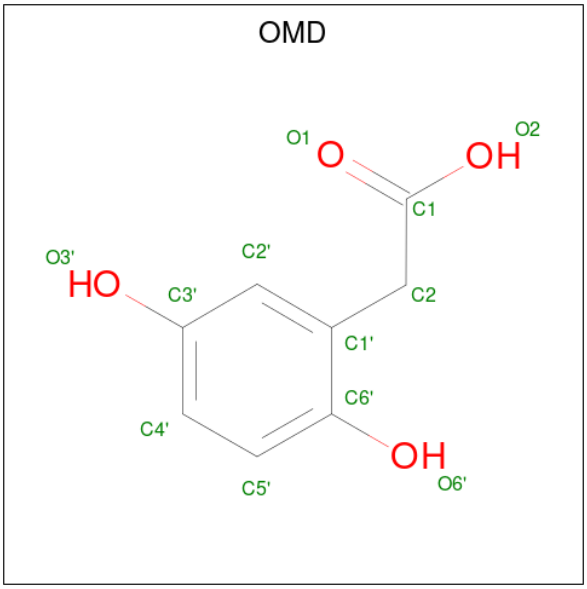
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	J	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0

- Molecule 3 is 4-Maleylacetoacetic acid (three-letter code: M8O) (formula: $C_8H_8O_6$).



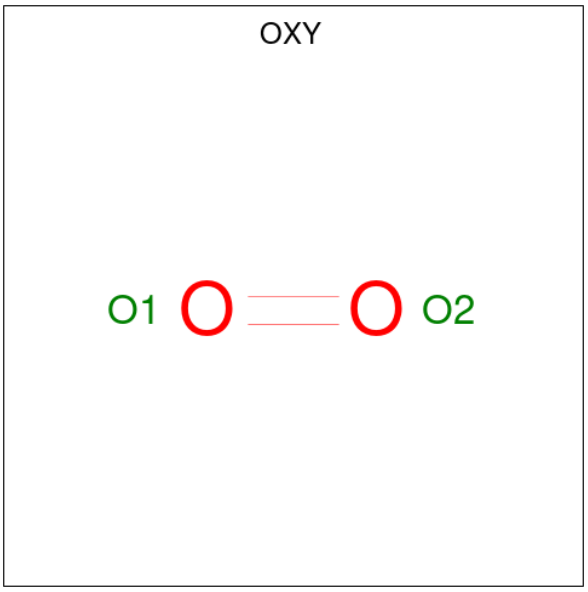
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 14 8 6	0	0

- Molecule 4 is 2-(3,6-DIHYDROXYPHENYL)ACETIC ACID (three-letter code: OMD) (formula: $C_8H_8O_4$).



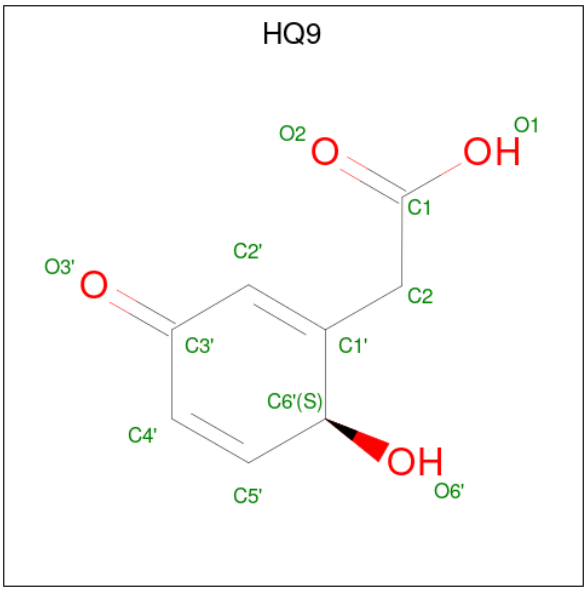
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 12 8 4	0	0
4	D	1	Total C O 12 8 4	0	0
4	E	1	Total C O 12 8 4	0	0
4	G	1	Total C O 12 8 4	0	0
4	H	1	Total C O 12 8 4	0	0
4	I	1	Total C O 12 8 4	0	0
4	J	1	Total C O 12 8 4	0	0
4	K	1	Total C O 12 8 4	0	0

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



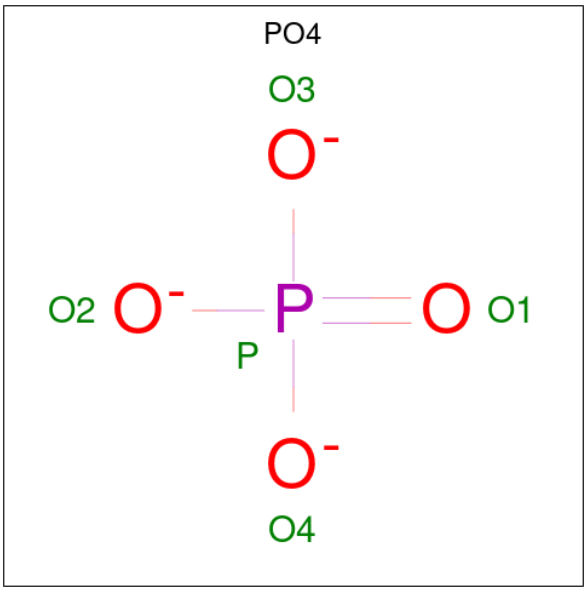
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O 2 2	0	0

- Molecule 6 is 2-(6-oxidanyl-3-oxidanylidene-cyclohexa-1,4-dien-1-yl)ethanoic acid (three-letter code: HQ9) (formula: $C_8H_8O_4$).



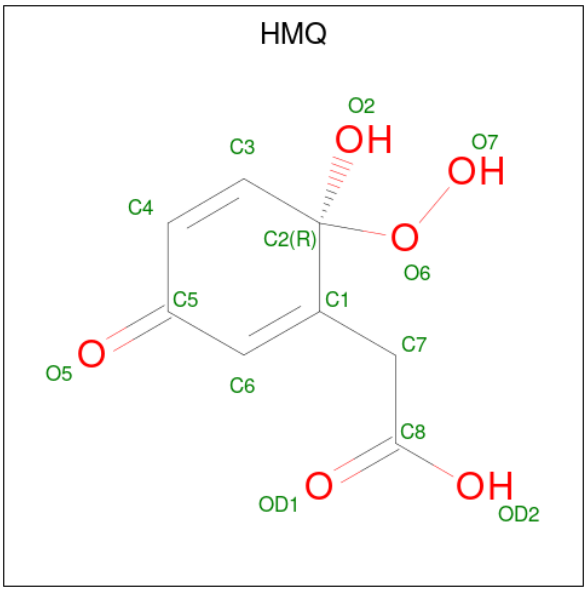
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 12 8 4	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total O P 5 4 1	0	0

- Molecule 8 is 2-[(6R)-6-(dioxidanyl)-6-oxidanyl-3-oxidanylidene-cyclohexa-1,4-dien-1-yl]ethanoic acid (three-letter code: HMQ) (formula: $C_8H_8O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total C O 14 8 6	0	0
8	L	1	Total C O 14 8 6	0	0

- Molecule 9 is water.

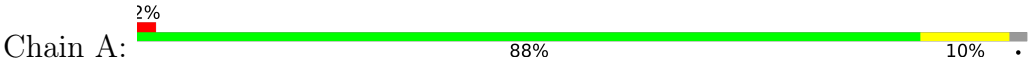
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	543	Total O 543 543	0	0
9	B	523	Total O 523 523	0	0
9	C	490	Total O 490 490	0	0
9	D	547	Total O 547 547	0	0
9	E	500	Total O 500 500	0	0
9	F	471	Total O 471 471	0	0
9	G	434	Total O 434 434	0	0
9	H	475	Total O 475 475	0	0
9	I	404	Total O 404 404	0	0
9	J	501	Total O 501 501	0	0
9	K	403	Total O 403 403	0	0
9	L	410	Total O 410 410	0	0

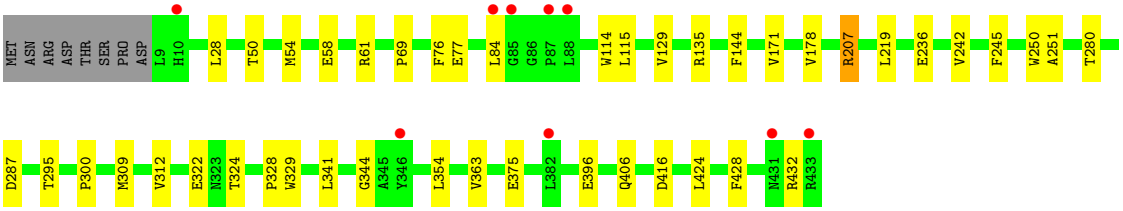
3 Residue-property plots

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: HOMOGENTISATE 1,2-DIOXYGENASE

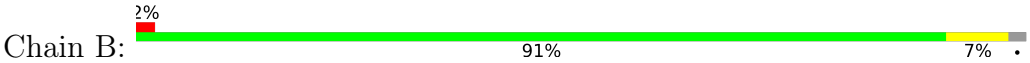
Chain A:

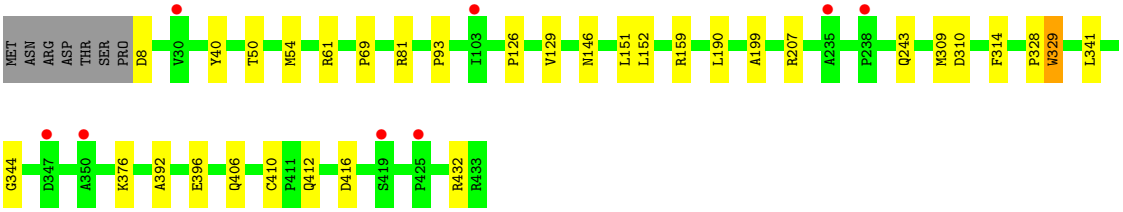




• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

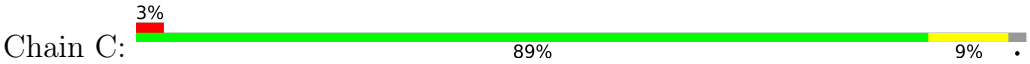
Chain B:

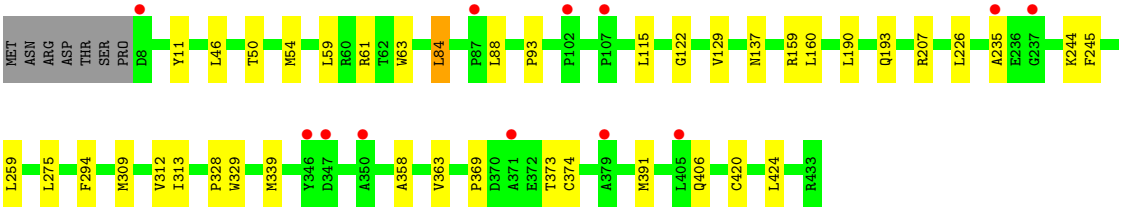




• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

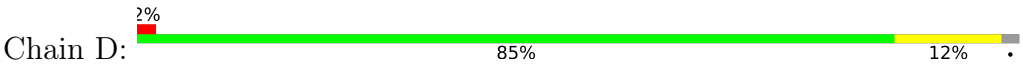
Chain C:

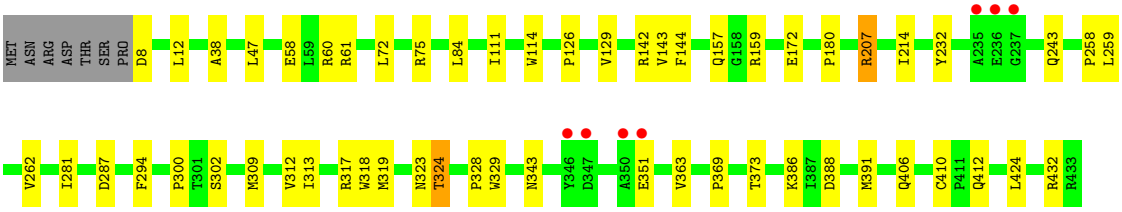




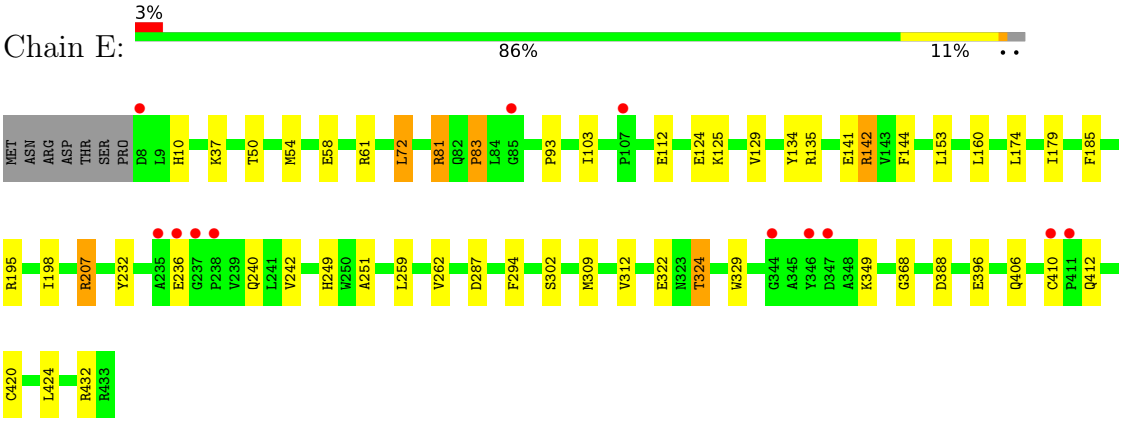
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain D:

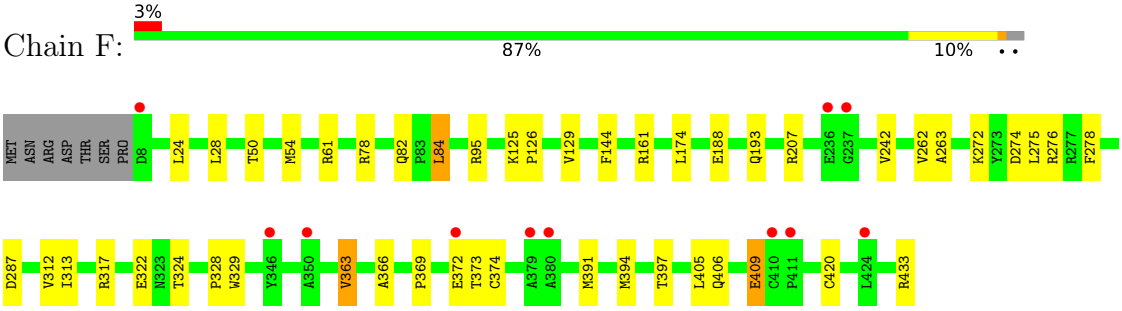




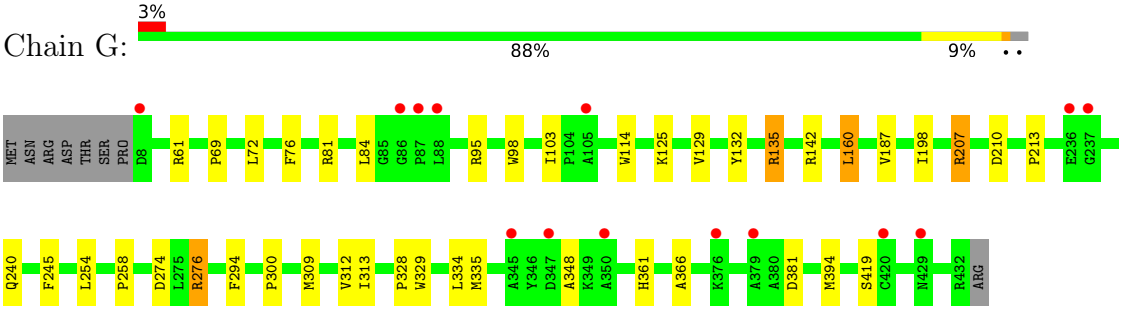
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



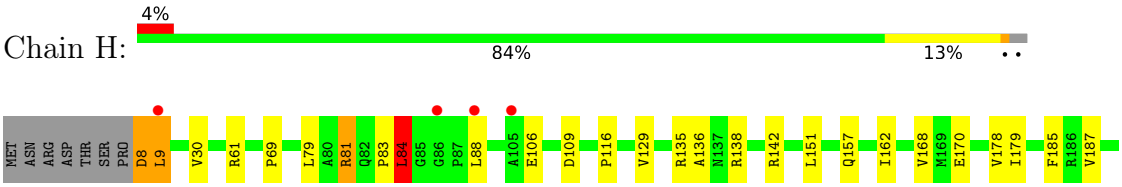
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

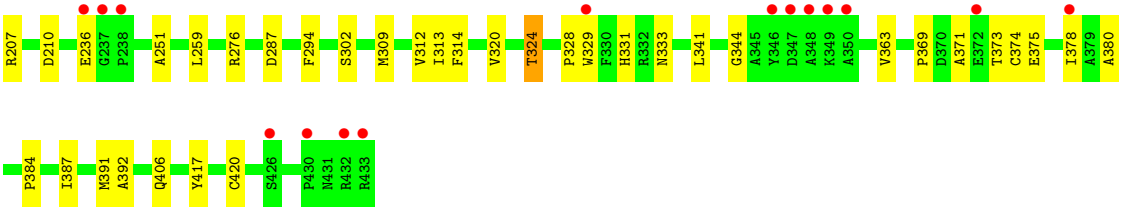


• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

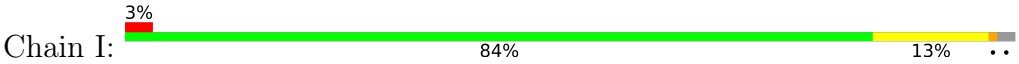


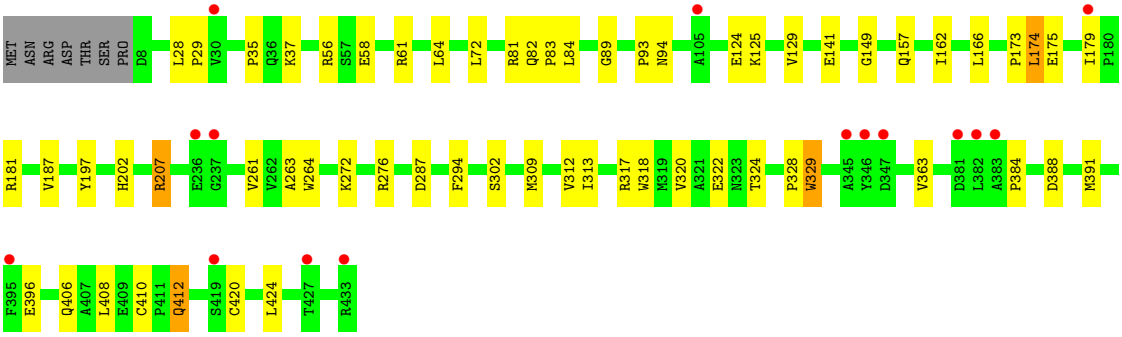
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



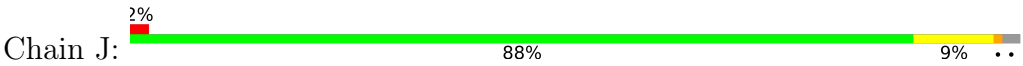


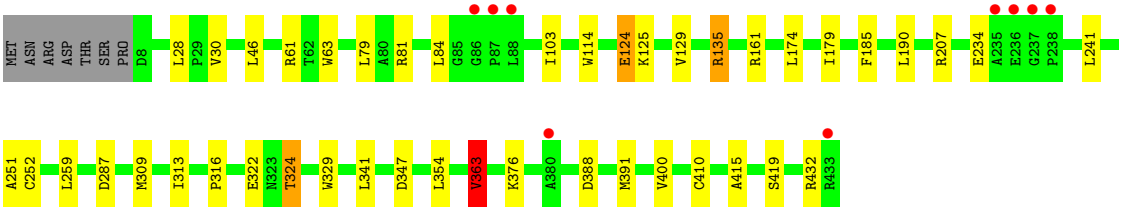
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



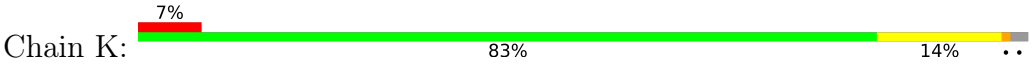


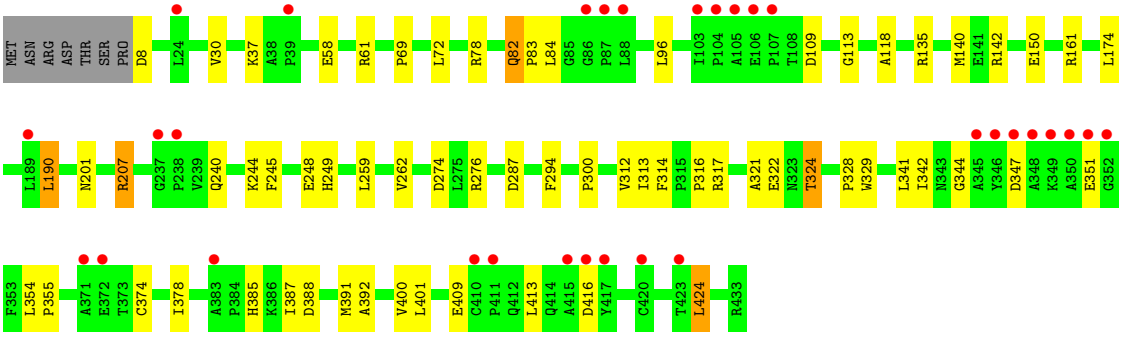
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



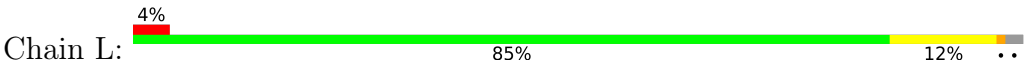


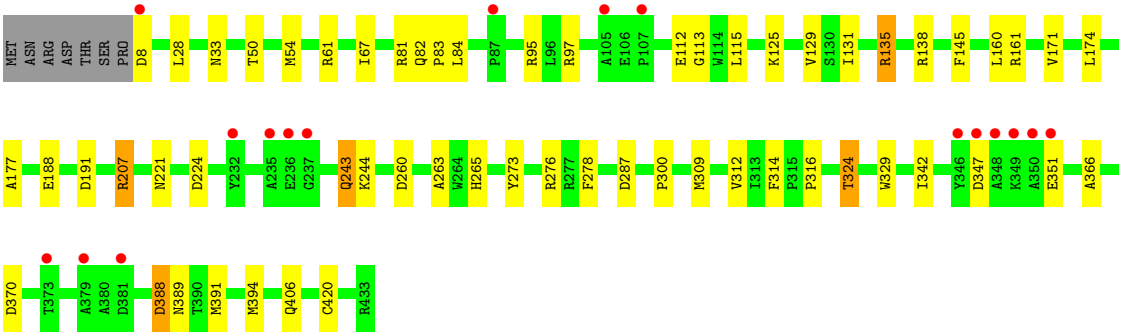
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE





• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE




MET
ASN
ARG
ASP
THR
SER
PRO
D8
L28
N33
T50
M54
R61
I67
R81
Q82
P83
L84
P87
R95
L96
R97
A105
E106
P107
E112
G113
W114
L115
K125
V129
S130
I131
R135
R138
F145
L160
R161
V171
L174
A177
E188
D191
R207
N221
D224
Y232
A235
E236
Q237
Q243
K244
D260
A263
W264
H265
Y273
R276
R277
F278
D287
P300
M309
V312
I313
F314
P315
P316
T324
W329
I342
Y346
D347
A348
K349
A350
E351
A366
D370
T373
A379
A380
D381
D388
N389
T390
M391
M394
Q406
C420
R433

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	93.74Å 93.86Å 163.44Å 87.62° 80.39° 68.29°	Depositor
Resolution (Å)	34.37 – 1.70 34.37 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.9 (34.37-1.70) 94.9 (34.37-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 1.70Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.203 , 0.252 0.225 , 0.225	Depositor DCC
R_{free} test set	26636 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	13.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 74.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	46082	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.25% 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: PO4, HQ9, OMD, FE, HMQ, M8O, OXY

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	0.53	0/3485	0.71	0/4746
1	B	0.52	0/3472	0.71	0/4729
1	C	0.54	0/3461	0.74	0/4716
1	D	0.54	0/3492	0.74	0/4756
1	E	0.56	3/3462 (0.1%)	0.75	2/4716 (0.0%)
1	F	0.53	0/3483	0.74	1/4743 (0.0%)
1	G	0.53	0/3450	0.72	0/4702
1	H	0.54	1/3451 (0.0%)	0.75	2/4702 (0.0%)
1	I	0.53	0/3440	0.73	1/4689 (0.0%)
1	J	0.56	0/3461	0.75	0/4715
1	K	0.51	0/3462	0.74	2/4716 (0.0%)
1	L	0.52	1/3434 (0.0%)	0.73	1/4680 (0.0%)
All	All	0.53	5/41553 (0.0%)	0.73	9/56610 (0.0%)

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	E	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	81[A]	ARG	CA-C	7.17	1.71	1.52
1	E	81[B]	ARG	CA-C	7.17	1.71	1.52
1	E	83	PRO	N-CD	5.37	1.55	1.47
1	L	83	PRO	N-CD	5.25	1.55	1.47
1	H	83	PRO	N-CD	5.07	1.54	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	84	LEU	CB-CG-CD2	6.70	122.38	111.00
1	K	82	GLN	C-N-CD	6.29	141.61	128.40
1	E	81[A]	ARG	CA-C-O	-6.26	106.95	120.10
1	E	81[B]	ARG	CA-C-O	-6.26	106.95	120.10
1	F	82	GLN	C-N-CD	5.59	140.13	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	81[A]	ARG	Mainchain
1	E	81[B]	ARG	Mainchain

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	3365	0	3291	26	0
1	B	3358	0	3276	18	0
1	C	3350	0	3261	20	0
1	D	3372	0	3300	29	0
1	E	3351	0	3267	26	0
1	F	3366	0	3297	27	0
1	G	3339	0	3254	23	0
1	H	3343	0	3254	31	0
1	I	3335	0	3241	43	0
1	J	3350	0	3269	21	0
1	K	3351	0	3266	40	0
1	L	3332	0	3236	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	14	0	6	2	0
4	B	12	0	5	2	0
4	D	12	0	5	0	0
4	E	12	0	5	0	0
4	G	12	0	5	0	0
4	H	12	0	5	0	0
4	I	12	0	6	2	0
4	J	12	0	5	0	0
4	K	12	0	5	1	0
5	C	2	0	0	2	0
6	C	12	0	6	2	0
7	E	5	0	0	0	0
8	F	14	0	6	1	0
8	L	14	0	7	1	0
9	A	543	0	0	9	0
9	B	523	0	0	3	0
9	C	490	0	0	1	0
9	D	547	0	0	10	0
9	E	500	0	0	4	0
9	F	471	0	0	5	0
9	G	434	0	0	3	0
9	H	475	0	0	6	0
9	I	404	0	0	13	0
9	J	501	0	0	3	0
9	K	403	0	0	4	1
9	L	410	0	0	7	1
All	All	46082	0	39278	322	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 322 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)
8:F:2001:HMQ:O7	8:F:2001:HMQ:O6	1.53	1.24
8:L:2001:HMQ:O7	8:L:2001:HMQ:O6	1.57	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:287:ASP:H	1:L:324:THR:HG21	1.21	1.05
1:E:287:ASP:H	1:E:324:THR:HG21	1.27	0.97
1:F:287:ASP:H	1:F:324:THR:HG21	1.31	0.95

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:3260:HOH:O	9:L:3057:HOH:O[1_644]	2.14	0.06

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	429/433 (99%)	417 (97%)	11 (3%)	1 (0%)	47	30
1	B	428/433 (99%)	414 (97%)	14 (3%)	0	100	100
1	C	427/433 (99%)	410 (96%)	16 (4%)	1 (0%)	47	30
1	D	430/433 (99%)	416 (97%)	13 (3%)	1 (0%)	47	30
1	E	427/433 (99%)	412 (96%)	14 (3%)	1 (0%)	47	30
1	F	429/433 (99%)	414 (96%)	14 (3%)	1 (0%)	47	30
1	G	426/433 (98%)	414 (97%)	12 (3%)	0	100	100
1	H	426/433 (98%)	411 (96%)	13 (3%)	2 (0%)	29	13
1	I	425/433 (98%)	416 (98%)	7 (2%)	2 (0%)	29	13
1	J	427/433 (99%)	410 (96%)	15 (4%)	2 (0%)	29	13
1	K	427/433 (99%)	410 (96%)	17 (4%)	0	100	100
1	L	424/433 (98%)	406 (96%)	18 (4%)	0	100	100
All	All	5125/5196 (99%)	4950 (97%)	164 (3%)	11 (0%)	47	30

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	235	ALA
1	E	174	LEU
1	F	363	VAL
1	I	174	LEU
1	H	380	ALA

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	353/355 (99%)	339 (96%)	14 (4%)	31 13
1	B	352/355 (99%)	341 (97%)	11 (3%)	40 21
1	C	351/355 (99%)	340 (97%)	11 (3%)	40 21
1	D	354/355 (100%)	334 (94%)	20 (6%)	21 7
1	E	351/355 (99%)	330 (94%)	21 (6%)	19 6
1	F	353/355 (99%)	339 (96%)	14 (4%)	31 13
1	G	350/355 (99%)	338 (97%)	12 (3%)	37 18
1	H	350/355 (99%)	329 (94%)	21 (6%)	19 6
1	I	349/355 (98%)	336 (96%)	13 (4%)	34 15
1	J	351/355 (99%)	334 (95%)	17 (5%)	25 9
1	K	351/355 (99%)	334 (95%)	17 (5%)	25 9
1	L	348/355 (98%)	330 (95%)	18 (5%)	23 8
All	All	4213/4260 (99%)	4024 (96%)	189 (4%)	28 10

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	236	GLU
1	J	207	ARG
1	H	324	THR
1	I	157	GLN

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Mol	Chain	Res	Type
1	J	376	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	10	HIS
1	K	240	GLN
1	K	406	GLN
1	D	343	ASN
1	D	323	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 12 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	OXY	C	1999	2	1,1,1	0.67	0	-		
4	OMD	K	2001	2	12,12,12	1.30	1 (8%)	16,16,16	1.56	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	HQ9	C	2001	2	10,12,12	2.46	4 (40%)	8,16,16	1.80	3 (37%)
4	OMD	I	2001	2	12,12,12	1.12	1 (8%)	16,16,16	2.09	5 (31%)
3	M8O	A	2001	2	12,13,13	3.17	5 (41%)	14,16,16	2.51	4 (28%)
7	PO4	E	2002	-	4,4,4	1.20	1 (25%)	6,6,6	0.40	0
8	HMQ	F	2001	2	11,14,14	2.11	5 (45%)	12,20,20	1.49	4 (33%)
4	OMD	H	2001	2	12,12,12	1.19	1 (8%)	16,16,16	2.12	6 (37%)
4	OMD	J	2001	2	12,12,12	1.16	1 (8%)	16,16,16	1.40	3 (18%)
4	OMD	E	2001	2	12,12,12	1.27	2 (16%)	16,16,16	2.11	5 (31%)
8	HMQ	L	2001	2	11,14,14	3.01	4 (36%)	12,20,20	2.58	6 (50%)
4	OMD	D	2001	2	12,12,12	1.77	4 (33%)	16,16,16	1.63	3 (18%)
4	OMD	G	2001	2	12,12,12	1.36	2 (16%)	16,16,16	1.33	2 (12%)
4	OMD	B	2001	2	12,12,12	1.46	2 (16%)	16,16,16	1.61	4 (25%)

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	OMD	K	2001	2	-	1/4/4/4	0/1/1/1
6	HQ9	C	2001	2	-	1/4/17/17	0/1/1/1
4	OMD	I	2001	2	-	2/4/4/4	0/1/1/1
3	M8O	A	2001	2	-	12/13/13/13	-
8	HMQ	F	2001	2	-	2/4/23/23	0/1/1/1
4	OMD	H	2001	2	-	0/4/4/4	0/1/1/1
4	OMD	J	2001	2	-	0/4/4/4	0/1/1/1
4	OMD	E	2001	2	-	0/4/4/4	0/1/1/1
8	HMQ	L	2001	2	-	2/4/23/23	0/1/1/1
4	OMD	D	2001	2	-	0/4/4/4	0/1/1/1
4	OMD	G	2001	2	-	0/4/4/4	0/1/1/1
4	OMD	B	2001	2	-	0/4/4/4	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	2001	HMQ	O2-C2	8.67	1.56	1.39
3	A	2001	M8O	O6-C50	8.46	1.37	1.23
6	C	2001	HQ9	O3'-C3'	5.80	1.42	1.24
8	F	2001	HMQ	C7-C8	4.34	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	M8O	C1-C3	4.18	1.58	1.48

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2001	M8O	O5-C5-C4	-6.99	108.99	120.83
4	I	2001	OMD	C4'-C3'-C2'	-4.78	114.94	120.17
4	E	2001	OMD	C4'-C3'-C2'	-4.74	114.98	120.17
8	L	2001	HMQ	C2-C1-C6	4.44	124.67	119.28
4	H	2001	OMD	C2-C1'-C6'	4.42	125.80	120.88

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	M8O	C3-C1-C7-C50
3	A	2001	M8O	O1-C2-C4-C5
3	A	2001	M8O	C2-C4-C5-O5
3	A	2001	M8O	O6-C50-C6-C5
3	A	2001	M8O	C7-C50-C6-C5

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1999	OXY	2	0
4	K	2001	OMD	1	0
6	C	2001	HQ9	2	0
4	I	2001	OMD	2	0
3	A	2001	M8O	2	0
8	F	2001	HMQ	1	0
8	L	2001	HMQ	1	0
4	B	2001	OMD	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	424/433 (97%)	0.09	9 (2%)	63	67	6, 14, 30, 50	5 (1%)
1	B	426/433 (98%)	0.07	8 (1%)	66	70	7, 15, 30, 54	5 (1%)
1	C	426/433 (98%)	0.07	12 (2%)	53	57	6, 15, 29, 44	7 (1%)
1	D	426/433 (98%)	0.06	7 (1%)	72	76	6, 14, 27, 46	5 (1%)
1	E	426/433 (98%)	0.14	12 (2%)	53	57	7, 16, 31, 53	4 (0%)
1	F	426/433 (98%)	0.22	11 (2%)	56	60	9, 17, 32, 50	5 (1%)
1	G	425/433 (98%)	0.13	14 (3%)	46	51	7, 14, 30, 55	4 (0%)
1	H	426/433 (98%)	0.28	19 (4%)	33	37	10, 18, 34, 56	4 (0%)
1	I	426/433 (98%)	0.27	15 (3%)	44	49	9, 18, 33, 52	6 (1%)
1	J	426/433 (98%)	0.13	9 (2%)	63	67	8, 16, 30, 49	5 (1%)
1	K	426/433 (98%)	0.53	31 (7%)	15	17	10, 20, 37, 58	7 (1%)
1	L	426/433 (98%)	0.32	17 (3%)	38	42	10, 19, 33, 49	6 (1%)
All	All	5109/5196 (98%)	0.19	164 (3%)	47	52	6, 17, 32, 58	63 (1%)

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	346	TYR	15.0
1	K	350	ALA	10.9
1	K	348	ALA	10.4
1	L	346	TYR	9.1
1	I	347	ASP	8.1

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	OMD	K	2001	12/12	0.82	0.32	9,13,18,19	12
4	OMD	J	2001	12/12	0.83	0.16	14,15,18,21	12
8	HMQ	L	2001	14/14	0.85	0.26	10,18,20,20	14
7	PO4	E	2002	5/5	0.86	0.21	41,44,44,45	5
4	OMD	D	2001	12/12	0.86	0.16	13,19,24,25	0
3	M8O	A	2001	14/14	0.87	0.17	7,20,25,30	14
8	HMQ	F	2001	14/14	0.90	0.15	11,16,20,23	14
4	OMD	H	2001	12/12	0.90	0.14	18,22,23,26	12
4	OMD	G	2001	12/12	0.91	0.12	15,18,20,23	0
4	OMD	E	2001	12/12	0.91	0.14	12,17,20,22	12
6	HQ9	C	2001	12/12	0.91	0.15	10,17,18,19	12
4	OMD	I	2001	12/12	0.92	0.16	12,22,25,26	12
4	OMD	B	2001	12/12	0.95	0.08	12,15,20,22	0
5	OXY	C	1999	2/2	0.97	0.14	7,7,7,14	2
2	FE	C	2000	1/1	0.99	0.04	10,10,10,10	0
2	FE	H	2000	1/1	0.99	0.02	14,14,14,14	0
2	FE	G	2000	1/1	1.00	0.03	10,10,10,10	0
2	FE	B	2000	1/1	1.00	0.03	8,8,8,8	1
2	FE	I	2000	1/1	1.00	0.03	15,15,15,15	0
2	FE	J	2000	1/1	1.00	0.05	13,13,13,13	0
2	FE	K	2000	1/1	1.00	0.03	14,14,14,14	0
2	FE	L	2000	1/1	1.00	0.04	13,13,13,13	0
2	FE	A	2000	1/1	1.00	0.05	11,11,11,11	0
2	FE	D	2000	1/1	1.00	0.03	11,11,11,11	0
2	FE	E	2000	1/1	1.00	0.03	12,12,12,12	0
2	FE	F	2000	1/1	1.00	0.05	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.