



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:34 PM GMT

PDB ID : 1PN2
Title : Crystal structure analysis of the selenomethionine labelled 2-enoyl-CoA hydratase 2 domain of Candida tropicalis multifunctional enzyme type 2
Authors : Koski, M.K.; Haapalainen, A.M.; Hiltunen, J.K.; Glumoff, T.
Deposited on : 2003-06-12
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

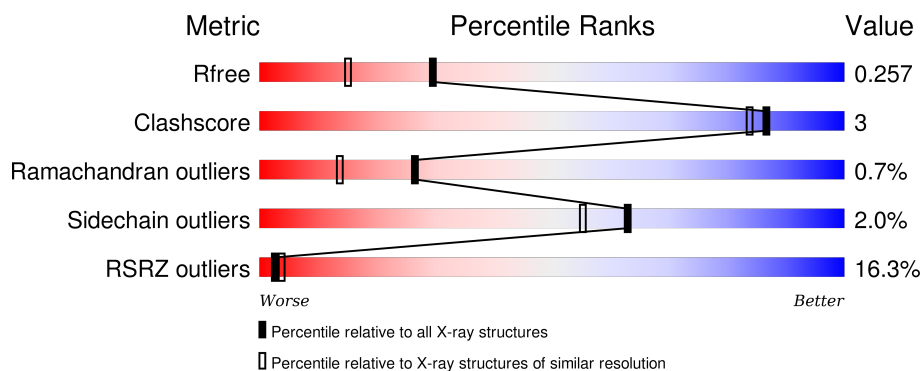
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	280	<div> <div>21%</div> <div>83%</div> <div>13%</div> <div>• •</div> </div>
1	B	280	<div> <div>16%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	C	280	<div> <div>14%</div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div>
1	D	280	<div> <div>11%</div> <div>86%</div> <div>10%</div> <div>•</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	805	-	-	-	X
2	EDO	C	801	-	-	-	X
2	EDO	C	803	-	-	-	X
2	EDO	D	802	-	-	-	X
2	EDO	D	804	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9374 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 Peroxisomal hydratase-dehydrogenase-epimerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	Se	98	0	0
			2153	1386	367	395	2	3			
1	B	270	Total	C	N	O	S	Se	51	0	0
			2141	1380	365	391	2	3			
1	C	267	Total	C	N	O	S	Se	36	0	0
			2117	1366	360	386	2	3			
1	D	272	Total	C	N	O	S	Se	32	0	0
			2153	1386	367	395	2	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	GLU	ENGINEERED	UNP P22414
A	69	MSE	MET	MODIFIED RESIDUE	UNP P22414
A	206	MSE	MET	MODIFIED RESIDUE	UNP P22414
A	222	MSE	MET	MODIFIED RESIDUE	UNP P22414
B	1	MSE	GLU	ENGINEERED	UNP P22414
B	69	MSE	MET	MODIFIED RESIDUE	UNP P22414
B	206	MSE	MET	MODIFIED RESIDUE	UNP P22414
B	222	MSE	MET	MODIFIED RESIDUE	UNP P22414
C	1	MSE	GLU	ENGINEERED	UNP P22414
C	69	MSE	MET	MODIFIED RESIDUE	UNP P22414
C	206	MSE	MET	MODIFIED RESIDUE	UNP P22414
C	222	MSE	MET	MODIFIED RESIDUE	UNP P22414
D	1	MSE	GLU	ENGINEERED	UNP P22414
D	69	MSE	MET	MODIFIED RESIDUE	UNP P22414
D	206	MSE	MET	MODIFIED RESIDUE	UNP P22414
D	222	MSE	MET	MODIFIED RESIDUE	UNP P22414

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

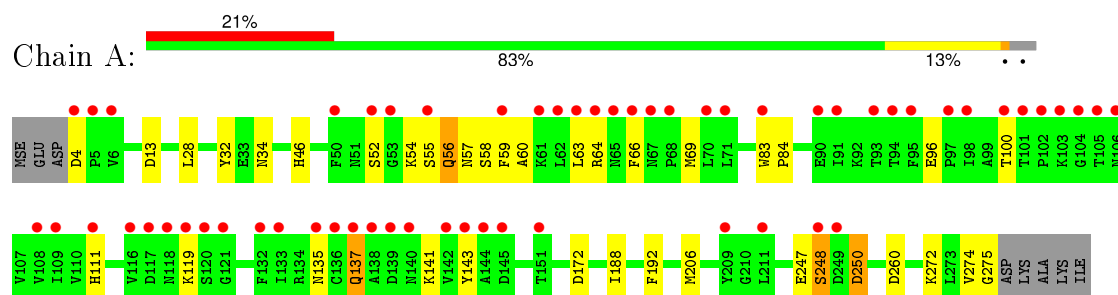
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	0
			153	153		
3	B	147	Total	O	0	0
			147	147		
3	C	236	Total	O	0	0
			236	236		
3	D	254	Total	O	0	0
			254	254		

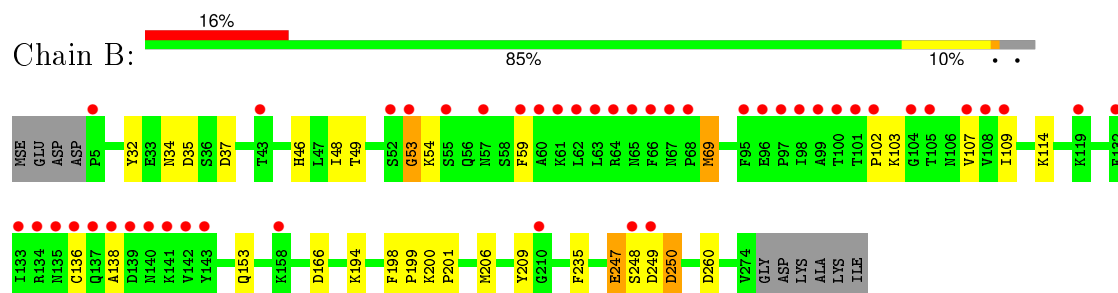
3 Residue-property plots

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

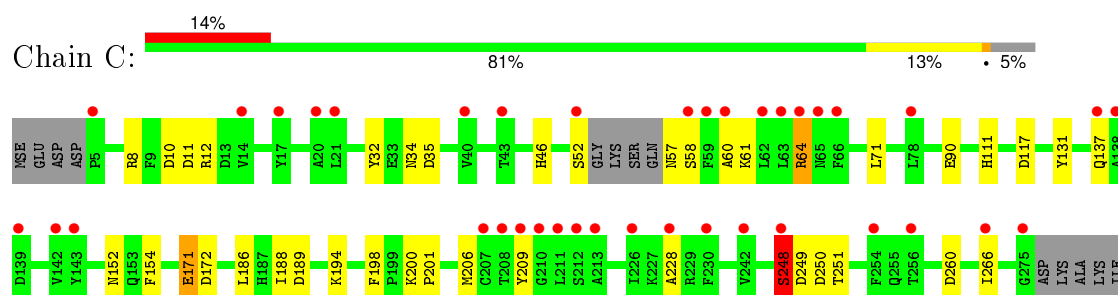
- Molecule 1: Peroxisomal hydratase-dehydrogenase-epimerase



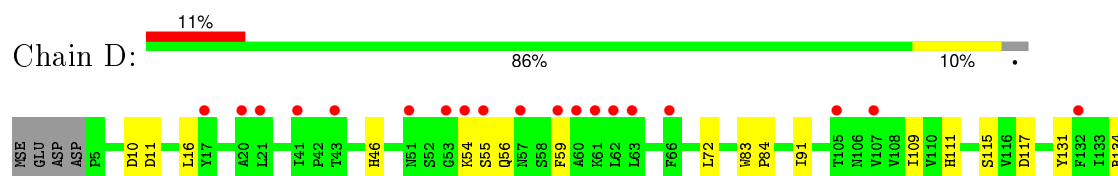
- Molecule 1: Peroxisomal hydratase-dehydrogenase-epimerase

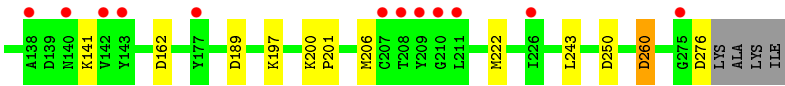


- Molecule 1: Peroxisomal hydratase-dehydrogenase-epimerase



- Molecule 1: Peroxisomal hydratase-dehydrogenase-epimerase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.80Å 60.65Å 131.12Å 90.00° 94.57° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 29.57 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-1.95) 95.2 (29.57-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.179 , 0.214 0.235 , 0.257	Depositor DCC
R_{free} test set	9759 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 97595 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9374	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.94	9/2207 (0.4%)	1.08	17/2996 (0.6%)
1	B	0.68	3/2195 (0.1%)	0.85	6/2979 (0.2%)
1	C	1.00	6/2170 (0.3%)	1.02	13/2945 (0.4%)
1	D	0.81	3/2207 (0.1%)	0.92	12/2995 (0.4%)
All	All	0.87	21/8779 (0.2%)	0.97	48/11915 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	GLU	CD-OE1	-22.05	1.01	1.25
1	C	61	LYS	CA-CB	-14.98	1.21	1.53
1	C	171	GLU	CD-OE2	-14.30	1.09	1.25
1	A	56	GLN	C-N	-10.74	1.09	1.34
1	C	171	GLU	CD-OE1	10.44	1.37	1.25
1	C	60	ALA	CA-CB	-9.83	1.31	1.52
1	A	60	ALA	C-N	-9.35	1.12	1.34
1	B	114	LYS	CE-NZ	-9.14	1.26	1.49
1	D	134	ARG	NE-CZ	-9.05	1.21	1.33
1	A	135	ASN	CA-CB	-7.81	1.32	1.53
1	C	52	SER	CA-CB	-7.26	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	SER	CB-OG	-7.13	1.32	1.42
1	B	103	LYS	CB-CG	-6.50	1.34	1.52
1	D	141	LYS	CD-CE	-6.33	1.35	1.51
1	B	249	ASP	CA-CB	-6.10	1.40	1.53
1	A	272	LYS	CD-CE	6.04	1.66	1.51
1	A	96	GLU	CD-OE2	6.03	1.32	1.25
1	A	100	THR	CA-CB	-5.60	1.38	1.53
1	C	249	ASP	CG-OD1	5.47	1.38	1.25
1	A	137	GLN	CA-CB	5.12	1.65	1.53
1	D	222	MSE	SE-CE	-5.12	1.65	1.95

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ASP	CB-CG-OD2	14.50	131.35	118.30
1	A	60	ALA	C-N-CA	14.40	157.70	121.70
1	A	96	GLU	OE1-CD-OE2	14.06	140.18	123.30
1	A	56	GLN	O-C-N	-13.59	100.96	122.70
1	C	60	ALA	N-CA-CB	-10.41	95.52	110.10
1	A	135	ASN	CB-CA-C	10.08	130.56	110.40
1	C	57	ASN	CB-CA-C	-9.89	90.63	110.40
1	A	60	ALA	O-C-N	-9.61	107.33	122.70
1	A	56	GLN	CA-C-N	8.59	136.11	117.20
1	C	60	ALA	CB-CA-C	8.32	122.58	110.10
1	A	96	GLU	CG-CD-OE2	-8.10	102.10	118.30
1	D	54	LYS	CB-CA-C	-7.45	95.50	110.40
1	C	10	ASP	CB-CG-OD2	7.38	124.95	118.30
1	B	53	GLY	N-CA-C	7.17	131.02	113.10
1	C	189	ASP	CB-CG-OD2	7.15	124.74	118.30
1	A	250	ASP	CB-CG-OD2	6.78	124.40	118.30
1	D	11	ASP	CB-CG-OD1	6.49	124.14	118.30
1	C	117	ASP	CB-CG-OD2	6.48	124.13	118.30
1	C	250	ASP	CB-CG-OD2	6.45	124.10	118.30
1	C	61	LYS	CB-CA-C	6.42	123.23	110.40
1	A	143	TYR	CB-CA-C	-6.37	97.65	110.40
1	D	10	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	119	LYS	CA-CB-CG	6.22	127.08	113.40
1	A	57	ASN	CB-CA-C	-6.20	98.01	110.40
1	A	4	ASP	CB-CG-OD2	5.90	123.61	118.30
1	D	134	ARG	CD-NE-CZ	5.90	131.86	123.60
1	D	134	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	D	260	ASP	CB-CG-OD2	5.84	123.56	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	TYR	CA-CB-CG	5.84	124.49	113.40
1	C	172	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	60	ALA	CA-C-N	5.75	129.84	117.20
1	B	103	LYS	CA-CB-CG	5.66	125.85	113.40
1	A	13	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	55	SER	CB-CA-C	-5.58	99.49	110.10
1	D	162	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	209	TYR	CA-CB-CG	5.55	123.95	113.40
1	D	276	ASP	CB-CG-OD2	5.48	123.23	118.30
1	D	134	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	B	166	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	56	GLN	C-N-CA	5.38	135.16	121.70
1	A	56	GLN	CB-CA-C	-5.32	99.76	110.40
1	D	189	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	117	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	37	ASP	CB-CG-OD2	5.26	123.04	118.30
1	C	35	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	11	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	250	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	35	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	GLN	Mainchain
1	B	250	ASP	Peptide
1	C	248	SER	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	2153	0	2131	11	0
1	B	2141	0	2127	13	0
1	C	2117	0	2100	13	0
1	D	2153	0	2134	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	6	1	0
2	C	8	0	12	0	0
2	D	8	0	12	0	0
3	A	153	0	0	0	0
3	B	147	0	0	1	0
3	C	236	0	0	0	0
3	D	254	0	0	0	0
All	All	9374	0	8522	45	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 3.

All (45) 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:54:LYS:O	1:A:58:SER:HB3	1.89	0.73
1:B:247:GLU:HA	1:B:247:GLU:OE1	1.91	0.69
1:C:58:SER:HB2	1:C:111:HIS:HE1	1.63	0.63
1:C:64:ARG:HB2	1:C:137:GLN:HB3	1.84	0.60
1:A:247:GLU:O	1:A:248:SER:HB3	2.02	0.59
1:C:12:ARG:HH21	1:D:16:LEU:HD23	1.69	0.58
1:C:32:TYR:CZ	1:C:34:ASN:HB2	2.40	0.56
1:B:69:MSE:HB2	3:B:402:HOH:O	2.05	0.56
1:D:46:HIS:CG	1:D:206:MSE:HE2	2.41	0.55
1:A:32:TYR:CZ	1:A:34:ASN:HB2	2.42	0.54
1:B:59:PHE:HB2	1:B:109:ILE:CD1	2.39	0.53
1:D:83:TRP:HB2	1:D:84:PRO:HA	1.94	0.50
1:B:48:ILE:HD12	1:B:49:THR:N	2.27	0.50
1:D:83:TRP:HA	1:D:84:PRO:C	2.32	0.50
1:B:107:VAL:HG12	1:B:136:CYS:HB3	1.93	0.50
1:A:172:ASP:OD2	2:A:805:EDO:O2	2.30	0.49
1:A:69:MSE:HE2	1:A:192:PHE:HB3	1.95	0.49
1:B:200:LYS:HB2	1:B:201:PRO:CD	2.43	0.48
1:A:46:HIS:CG	1:A:206:MSE:HE2	2.48	0.48
1:B:59:PHE:HB2	1:B:109:ILE:HD11	1.95	0.48
1:D:59:PHE:HB3	1:D:111:HIS:CD2	2.48	0.48
1:B:194:LYS:HA	1:B:198:PHE:O	2.13	0.47
1:C:46:HIS:CG	1:C:206:MSE:HE2	2.50	0.47
1:A:64:ARG:HB2	1:A:137:GLN:O	2.16	0.46
1:C:152:ASN:HB3	1:C:154:PHE:CE2	2.51	0.46
1:B:46:HIS:CG	1:B:206:MSE:HE2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ILE:HG23	1:D:131:TYR:HB2	1.98	0.45
1:C:58:SER:HB2	1:C:111:HIS:CE1	2.47	0.45
1:D:200:LYS:HB2	1:D:201:PRO:CD	2.48	0.44
1:A:63:LEU:HD23	1:A:66:PHE:CG	2.53	0.43
1:C:248:SER:HA	1:C:251:THR:H	1.83	0.43
1:C:8:ARG:NH1	1:C:90:GLU:OE2	2.52	0.43
1:C:71:LEU:HD11	1:C:131:TYR:HB3	2.00	0.42
1:B:102:PRO:HG3	1:B:138:ALA:O	2.19	0.42
1:D:91:ILE:CG2	1:D:115:SER:HB3	2.49	0.42
1:C:228:ALA:HB1	1:C:266:ILE:HG23	2.01	0.42
1:A:59:PHE:HB3	1:A:111:HIS:CD2	2.55	0.42
1:B:200:LYS:HB2	1:B:201:PRO:HD2	2.02	0.42
1:A:274:VAL:HG12	1:A:275:GLY:N	2.35	0.42
1:A:83:TRP:CG	1:A:84:PRO:HA	2.55	0.42
1:B:32:TYR:CZ	1:B:34:ASN:HB2	2.55	0.42
1:B:199:PRO:HG2	1:B:235:PHE:CZ	2.55	0.41
1:D:91:ILE:HG21	1:D:115:SER:HB3	2.03	0.41
1:C:194:LYS:HA	1:C:198:PHE:O	2.21	0.40
1:C:200:LYS:HB2	1:C:201:PRO:CD	2.51	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	270/280 (96%)	263 (97%)	5 (2%)	2 (1%)	26	14
1	B	268/280 (96%)	259 (97%)	7 (3%)	2 (1%)	26	14
1	C	263/280 (94%)	257 (98%)	4 (2%)	2 (1%)	24	11
1	D	270/280 (96%)	265 (98%)	4 (2%)	1 (0%)	39	27
All	All	1071/1120 (96%)	1044 (98%)	20 (2%)	7 (1%)	26	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	SER
1	B	53	GLY
1	B	54	LYS
1	C	248	SER
1	D	55	SER
1	C	188	ILE
1	A	188	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	233/236 (99%)	229 (98%)	4 (2%)	68	63
1	B	232/236 (98%)	226 (97%)	6 (3%)	54	43
1	C	229/236 (97%)	225 (98%)	4 (2%)	68	63
1	D	233/236 (99%)	228 (98%)	5 (2%)	61	53
All	All	927/944 (98%)	908 (98%)	19 (2%)	63	55

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	141	LYS
1	A	250	ASP
1	A	260	ASP
1	B	69	MSE
1	B	153	GLN
1	B	247	GLU
1	B	248	SER
1	B	250	ASP
1	B	260	ASP
1	C	64	ARG
1	C	171	GLU
1	C	186	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	260	ASP
1	D	56	GLN
1	D	72	LEU
1	D	197	LYS
1	D	243	LEU
1	D	260	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	111	HIS
1	C	111	HIS
1	C	140	ASN
1	D	111	HIS
1	D	140	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	EDO	A	805	-	3,3,3	0.42	0	2,2,2	0.03	0
2	EDO	C	801	-	3,3,3	0.26	0	2,2,2	1.20	0
2	EDO	C	803	-	3,3,3	0.21	0	2,2,2	0.55	0
2	EDO	D	802	-	3,3,3	0.51	0	2,2,2	0.23	0
2	EDO	D	804	-	3,3,3	0.29	0	2,2,2	0.79	0

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	EDO	A	805	-	-	0/1/1/1	0/0/0/0
2	EDO	C	801	-	-	0/1/1/1	0/0/0/0
2	EDO	C	803	-	-	0/1/1/1	0/0/0/0
2	EDO	D	802	-	-	0/1/1/1	0/0/0/0
2	EDO	D	804	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	805	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	267/280 (95%)	1.01	59 (22%) 1 1	2, 6, 22, 27	27 (10%)
1	B	267/280 (95%)	0.67	46 (17%) 2 3	2, 6, 21, 37	16 (5%)
1	C	264/280 (94%)	0.64	38 (14%) 3 6	2, 6, 26, 41	13 (4%)
1	D	269/280 (96%)	0.57	31 (11%) 6 11	2, 6, 21, 53	10 (3%)
All	All	1067/1120 (95%)	0.72	174 (16%) 2 4	2, 6, 23, 53	66 (6%)

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	CYS	7.1
1	A	63	LEU	6.3
1	A	144	ALA	6.1
1	A	108	VAL	6.0
1	A	100	THR	5.9
1	D	53	GLY	5.8
1	A	71	LEU	5.8
1	C	62	LEU	5.8
1	A	65	ASN	5.6
1	A	59	PHE	5.6
1	B	65	ASN	5.5
1	A	66	PHE	5.4
1	A	102	PRO	5.3
1	A	133	ILE	5.2
1	A	104	GLY	5.1
1	B	138	ALA	5.1
1	B	66	PHE	5.1
1	D	54	LYS	5.0
1	A	97	PRO	5.0
1	B	52	SER	4.8
1	A	249	ASP	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	140	ASN	4.4
1	B	63	LEU	4.4
1	A	53	GLY	4.3
1	B	62	LEU	4.3
1	B	143	TYR	4.2
1	A	4	ASP	4.2
1	A	139	ASP	4.2
1	D	62	LEU	4.2
1	A	5	PRO	4.1
1	B	68	PRO	4.0
1	B	59	PHE	4.0
1	B	53	GLY	4.0
1	A	137	GLN	3.9
1	A	145	ASP	3.9
1	B	101	THR	3.9
1	B	135	ASN	3.9
1	A	142	VAL	3.9
1	A	111	HIS	3.9
1	A	118	ASN	3.7
1	D	105	THR	3.7
1	C	66	PHE	3.7
1	B	99	ALA	3.7
1	A	105	THR	3.6
1	C	59	PHE	3.6
1	A	70	LEU	3.6
1	C	209	TYR	3.6
1	B	105	THR	3.6
1	B	102	PRO	3.6
1	C	266	ILE	3.5
1	B	60	ALA	3.5
1	B	100	THR	3.5
1	B	97	PRO	3.4
1	C	211	LEU	3.4
1	D	132	PHE	3.4
1	B	107	VAL	3.4
1	A	95	PHE	3.4
1	C	207	CYS	3.4
1	A	116	VAL	3.4
1	A	62	LEU	3.3
1	B	136	CYS	3.3
1	C	58	SER	3.3
1	B	95	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	132	PHE	3.3
1	B	98	ILE	3.3
1	A	68	PRO	3.3
1	D	21	LEU	3.2
1	D	143	TYR	3.2
1	D	209	TYR	3.2
1	C	210	GLY	3.2
1	C	5	PRO	3.2
1	B	61	LYS	3.2
1	C	275	GLY	3.2
1	C	63	LEU	3.2
1	A	132	PHE	3.2
1	A	106	ASN	3.2
1	A	143	TYR	3.1
1	A	121	GLY	3.1
1	D	211	LEU	3.1
1	A	64	ARG	3.1
1	A	98	ILE	3.1
1	B	133	ILE	3.0
1	B	137	GLN	3.0
1	A	61	LYS	3.0
1	A	248	SER	3.0
1	D	138	ALA	3.0
1	B	109	ILE	3.0
1	C	208	THR	3.0
1	D	207	CYS	3.0
1	B	140	ASN	2.9
1	D	226	ILE	2.9
1	C	64	ARG	2.9
1	A	119	LYS	2.9
1	C	143	TYR	2.9
1	A	117	ASP	2.9
1	B	5	PRO	2.8
1	B	67	ASN	2.8
1	C	248	SER	2.8
1	D	57	ASN	2.7
1	C	226	ILE	2.7
1	D	41	ILE	2.7
1	D	275	GLY	2.7
1	A	94	THR	2.7
1	C	60	ALA	2.7
1	A	91	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	120	SER	2.7
1	C	230	PHE	2.7
1	B	104	GLY	2.7
1	B	249	ASP	2.7
1	A	109	ILE	2.6
1	C	228	ALA	2.6
1	D	60	ALA	2.6
1	A	90	GLU	2.6
1	C	52	SER	2.6
1	A	135	ASN	2.6
1	C	242	VAL	2.6
1	D	17	TYR	2.6
1	C	212	SER	2.6
1	B	158	LYS	2.5
1	B	248	SER	2.5
1	A	101	THR	2.5
1	A	138	ALA	2.5
1	D	55	SER	2.5
1	C	43	THR	2.5
1	D	210	GLY	2.5
1	A	6	VAL	2.4
1	D	43	THR	2.4
1	B	141	LYS	2.4
1	A	50	PHE	2.4
1	C	17	TYR	2.4
1	B	55	SER	2.4
1	A	103	LYS	2.4
1	C	21	LEU	2.4
1	B	57	ASN	2.4
1	B	108	VAL	2.4
1	A	93	THR	2.4
1	A	83	TRP	2.3
1	C	213	ALA	2.3
1	B	64	ARG	2.3
1	B	134	ARG	2.3
1	A	55	SER	2.3
1	C	138	ALA	2.3
1	C	139	ASP	2.2
1	B	119	LYS	2.2
1	C	20	ALA	2.2
1	A	52	SER	2.2
1	C	256	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	96	GLU	2.2
1	D	107	VAL	2.2
1	B	139	ASP	2.1
1	D	66	PHE	2.1
1	A	211	LEU	2.1
1	C	78	LEU	2.1
1	C	40	VAL	2.1
1	C	137	GLN	2.1
1	A	151	THR	2.1
1	A	67	ASN	2.1
1	D	51	ASN	2.1
1	D	177	TYR	2.1
1	D	61	LYS	2.1
1	B	142	VAL	2.1
1	D	63	LEU	2.1
1	C	14	VAL	2.1
1	C	254	PHE	2.1
1	D	59	PHE	2.1
1	A	209	TYR	2.1
1	C	142	VAL	2.1
1	D	142	VAL	2.1
1	C	65	ASN	2.0
1	D	20	ALA	2.0
1	B	210	GLY	2.0
1	D	140	ASN	2.0
1	B	43	THR	2.0
1	D	208	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	EDO	A	805	4/4	0.71	0.21	6.71	44,47,49,49	0
2	EDO	D	802	4/4	0.95	0.24	5.74	21,22,26,26	0
2	EDO	C	803	4/4	0.87	0.30	5.24	34,39,40,44	0
2	EDO	D	804	4/4	0.88	0.20	3.66	34,37,40,44	0
2	EDO	C	801	4/4	0.95	0.26	2.74	29,33,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.