



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 07:35 AM EDT

PDB ID : 6TFR  
Title : Linalool Dehydratase Isomerase C180A mutant  
Authors : Cuetos, A.; Zukic, E.; Danesh-Azari, H.R.; Grogan, G.  
Deposited on : 2019-11-14  
Resolution : 1.45 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.37.1  
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) : 2.37.1

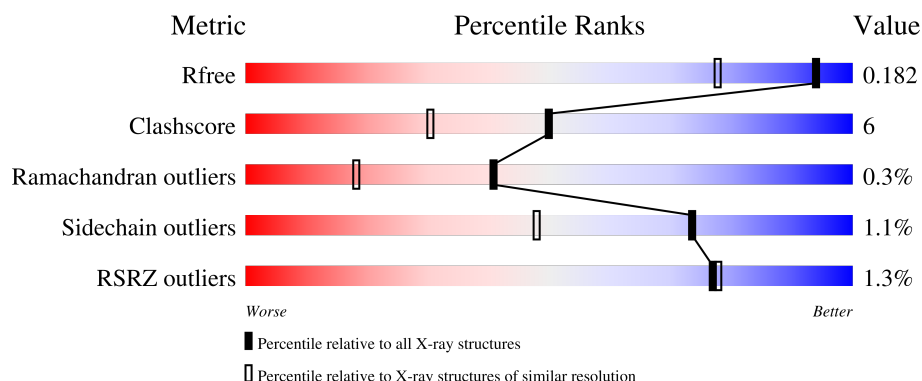
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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  $\geq 3$ , 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	373	<div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	B	373	<div> <div>91%</div> <div>7%</div> <div>..</div> </div>
1	C	373	<div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	D	373	<div> <div>90%</div> <div>6%</div> <div>..</div> </div>
1	E	373	<div> <div>2%</div> <div>88%</div> <div>8%</div> <div>...</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16899 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 Linalool dehydratase-isomerase protein LDI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	10	0
			2944	1901	492	537	14			
1	B	368	Total	C	N	O	S	0	8	0
			2976	1918	499	544	15			
1	C	364	Total	C	N	O	S	0	11	0
			2966	1915	498	539	14			
1	D	364	Total	C	N	O	S	0	11	0
			2955	1909	495	537	14			
1	E	363	Total	C	N	O	S	0	8	0
			2937	1897	493	533	14			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP W8X534
A	1	MET	-	expression tag	UNP W8X534
A	180	ALA	CYS	engineered mutation	UNP W8X534
B	0	ALA	-	expression tag	UNP W8X534
B	1	MET	-	expression tag	UNP W8X534
B	180	ALA	CYS	engineered mutation	UNP W8X534
C	0	ALA	-	expression tag	UNP W8X534
C	1	MET	-	expression tag	UNP W8X534
C	180	ALA	CYS	engineered mutation	UNP W8X534
D	0	ALA	-	expression tag	UNP W8X534
D	1	MET	-	expression tag	UNP W8X534
D	180	ALA	CYS	engineered mutation	UNP W8X534
E	0	ALA	-	expression tag	UNP W8X534
E	1	MET	-	expression tag	UNP W8X534
E	180	ALA	CYS	engineered mutation	UNP W8X534

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	380	Total O 380 380	0	0
3	B	442	Total O 442 442	0	0

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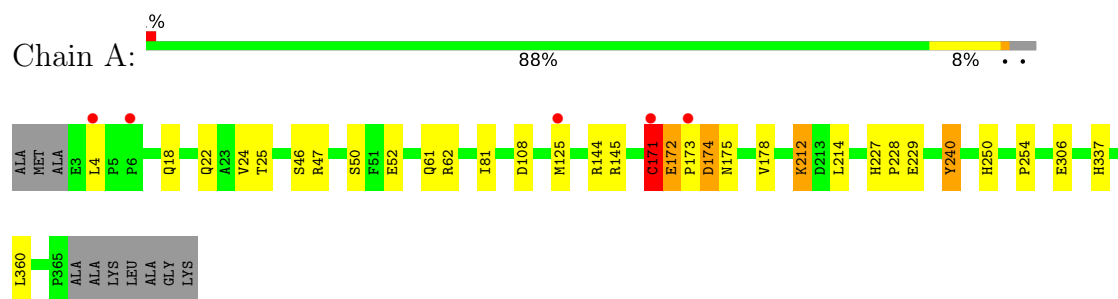
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	417	Total 417	O 417	0	0
3	D	446	Total 446	O 446	0	0
3	E	396	Total 396	O 396	0	0

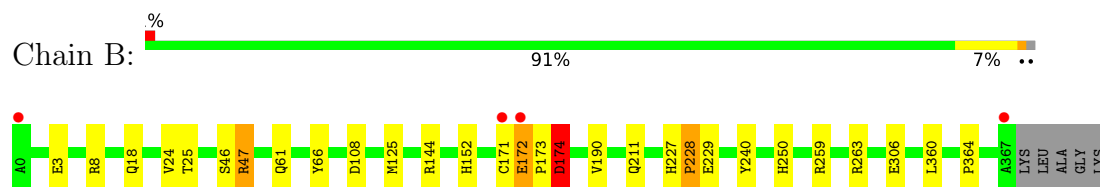
### 3 Residue-property plots [i](#)

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.

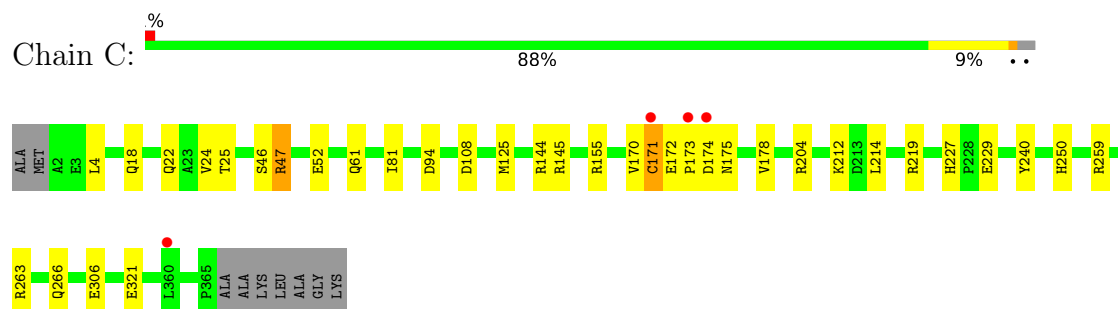
- Molecule 1: Linalool dehydratase-isomerase protein LDI



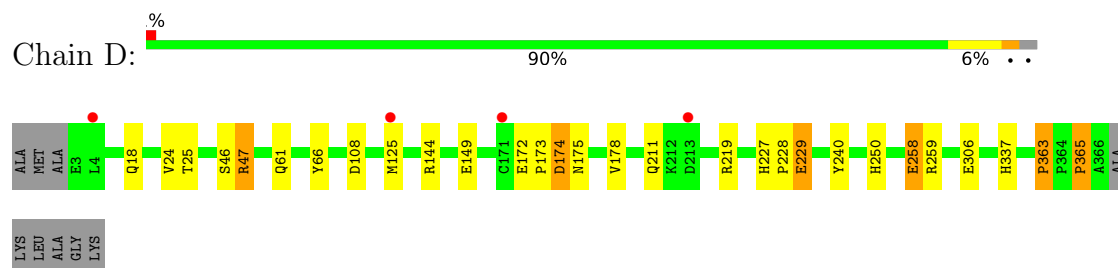
- Molecule 1: Linalool dehydratase-isomerase protein LDI



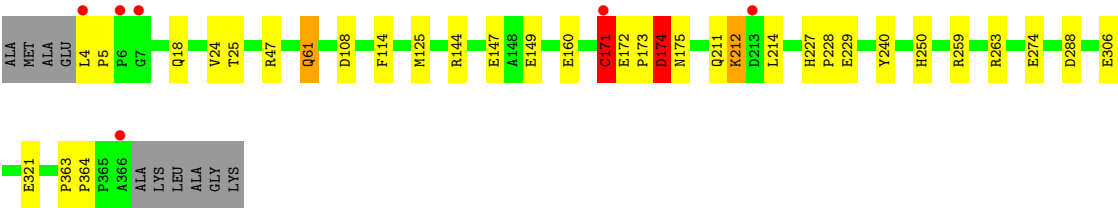
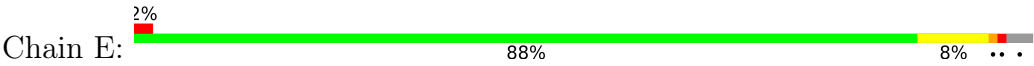
- Molecule 1: Linalool dehydratase-isomerase protein LDI



- Molecule 1: Linalool dehydratase-isomerase protein LDI



● Molecule 1: Linalool dehydratase-isomerase protein LDI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.44Å 106.97Å 123.67Å 90.00° 95.97° 90.00°	Depositor
Resolution (Å)	55.32 – 1.45 55.32 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.32-1.45) 99.9 (55.32-1.45)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.157 , 0.176 0.164 , 0.182	Depositor DCC
$R_{free}$ test set	18367 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16899	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.85	5/3049 (0.2%)	0.98	14/4149 (0.3%)
1	B	0.88	5/3072 (0.2%)	1.01	17/4178 (0.4%)
1	C	0.86	3/3071 (0.1%)	0.99	8/4177 (0.2%)
1	D	0.91	6/3060 (0.2%)	1.01	15/4164 (0.4%)
1	E	0.86	5/3036 (0.2%)	0.95	8/4131 (0.2%)
All	All	0.87	24/15288 (0.2%)	0.99	62/20799 (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	A	0	1
1	E	0	3
All	All	0	4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	365	PRO	N-CA	12.44	1.68	1.47
1	D	363	PRO	N-CA	11.75	1.67	1.47
1	B	172[A]	GLU	C-N	8.02	1.49	1.34
1	B	172[B]	GLU	C-N	8.02	1.49	1.34
1	A	172[A]	GLU	C-N	7.26	1.48	1.34
1	A	172[B]	GLU	C-N	7.26	1.48	1.34
1	B	364	PRO	C-N	7.13	1.47	1.34
1	A	171[A]	CYS	CA-C	6.94	1.71	1.52
1	A	171[B]	CYS	CA-C	6.94	1.71	1.52
1	C	171[A]	CYS	C-N	-6.32	1.19	1.34
1	C	171[B]	CYS	C-N	-6.32	1.19	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	321	GLU	CD-OE1	-5.91	1.19	1.25
1	C	321	GLU	CD-OE2	-5.60	1.19	1.25
1	D	258	GLU	CD-OE2	5.59	1.31	1.25
1	E	149	GLU	CD-OE2	-5.44	1.19	1.25
1	B	174[A]	ASP	CG-OD2	5.44	1.37	1.25
1	B	174[B]	ASP	CG-OD2	5.44	1.37	1.25
1	E	174[A]	ASP	CG-OD2	5.37	1.37	1.25
1	E	174[B]	ASP	CG-OD2	5.37	1.37	1.25
1	A	212	LYS	C-O	5.36	1.33	1.23
1	D	174[A]	ASP	CG-OD2	5.20	1.37	1.25
1	D	174[B]	ASP	CG-OD2	5.20	1.37	1.25
1	E	212	LYS	C-O	5.07	1.32	1.23
1	D	149	GLU	CD-OE1	5.04	1.31	1.25

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	B	47[A]	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	B	47[B]	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	D	174[A]	ASP	CB-CG-OD2	8.07	125.56	118.30
1	D	174[B]	ASP	CB-CG-OD2	8.07	125.56	118.30
1	B	47[A]	ARG	CG-CD-NE	7.61	127.78	111.80
1	B	47[B]	ARG	CG-CD-NE	7.61	127.78	111.80
1	D	47	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	47[A]	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	B	47[B]	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	A	171[A]	CYS	O-C-N	-7.35	110.94	122.70
1	A	171[B]	CYS	O-C-N	-7.35	110.94	122.70
1	B	144	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	A	171[A]	CYS	CA-C-N	7.17	132.98	117.20
1	A	171[B]	CYS	CA-C-N	7.17	132.98	117.20
1	A	174[A]	ASP	CA-C-O	-7.07	105.25	120.10
1	A	174[B]	ASP	CA-C-O	-7.07	105.25	120.10
1	E	174[A]	ASP	CA-C-O	-6.96	105.49	120.10
1	E	174[B]	ASP	CA-C-O	-6.96	105.49	120.10
1	C	47[A]	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	C	47[B]	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	C	47[A]	ARG	CG-CD-NE	6.89	126.27	111.80
1	C	47[B]	ARG	CG-CD-NE	6.89	126.27	111.80
1	C	259	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	B	172[A]	GLU	N-CA-CB	6.54	122.37	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172[B]	GLU	N-CA-CB	6.54	122.37	110.60
1	B	172[A]	GLU	CB-CA-C	-6.46	97.48	110.40
1	B	172[B]	GLU	CB-CA-C	-6.46	97.48	110.40
1	D	363	PRO	N-CA-C	-6.36	95.56	112.10
1	D	144	ARG	NE-CZ-NH2	6.35	123.48	120.30
1	A	46	SER	N-CA-CB	-6.33	101.01	110.50
1	C	259	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	D	365	PRO	CA-N-CD	-6.19	102.83	111.50
1	E	171[A]	CYS	O-C-N	-6.19	112.80	122.70
1	E	171[B]	CYS	O-C-N	-6.19	112.80	122.70
1	B	8	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	D	219[A]	ARG	CB-CG-CD	6.07	127.38	111.60
1	D	219[B]	ARG	CB-CG-CD	6.07	127.38	111.60
1	D	144	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	D	174[A]	ASP	CA-C-O	-6.05	107.39	120.10
1	D	174[B]	ASP	CA-C-O	-6.05	107.39	120.10
1	B	174[A]	ASP	CA-C-O	-5.78	107.96	120.10
1	B	174[B]	ASP	CA-C-O	-5.78	107.96	120.10
1	C	46	SER	N-CA-CB	-5.74	101.89	110.50
1	A	174[A]	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	174[B]	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	46	SER	N-CA-CB	-5.70	101.95	110.50
1	D	363	PRO	CA-N-CD	-5.63	103.62	111.50
1	D	219[A]	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	D	219[B]	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	B	144	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	46	SER	N-CA-CB	-5.48	102.28	110.50
1	A	172[A]	GLU	O-C-N	-5.34	110.94	121.10
1	A	172[B]	GLU	O-C-N	-5.34	110.94	121.10
1	A	62	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	364	PRO	O-C-N	-5.15	111.31	121.10
1	A	144	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	E	144	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	E	174[A]	ASP	CB-CG-OD2	5.04	122.83	118.30
1	E	174[B]	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	240	TYR	CB-CG-CD1	-5.01	118.00	121.00
1	E	288	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171[B]	CYS	Mainchain
1	E	171[A]	CYS	Mainchain
1	E	171[B]	CYS	Mainchain
1	E	174[B]	ASP	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	2944	0	2841	37	0
1	B	2976	0	2874	27	0
1	C	2966	0	2867	45	0
1	D	2955	0	2851	30	0
1	E	2937	0	2839	40	0
2	A	8	0	12	0	0
2	B	16	0	24	0	0
2	C	8	0	12	0	0
2	D	4	0	6	0	0
2	E	4	0	6	0	0
3	A	380	0	0	12	0
3	B	442	0	0	7	0
3	C	417	0	0	12	0
3	D	446	0	0	13	0
3	E	396	0	0	14	0
All	All	16899	0	14332	170	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 6.

All (170) 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:D:365:PRO:CA	1:D:365:PRO:N	1.68	1.47
1:C:214:LEU:HG	3:C:1051:HOH:O	1.21	1.27
1:A:173[A]:PRO:HB2	1:C:47[A]:ARG:NH2	1.50	1.24
1:D:125[B]:MET:HG2	3:D:576:HOH:O	1.39	1.20
1:A:125[B]:MET:HG2	3:A:575:HOH:O	1.41	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171[B]:CYS:SG	3:A:575:HOH:O	1.96	1.15
1:B:125[B]:MET:HG2	3:B:555:HOH:O	0.99	1.14
1:E:125[B]:MET:HB3	1:E:171[B]:CYS:SG	1.89	1.12
1:B:47[A]:ARG:NH1	1:E:173[A]:PRO:HB2	1.65	1.11
1:C:173[A]:PRO:HA	3:C:1006:HOH:O	1.53	1.06
1:C:125[B]:MET:HG2	1:C:171[B]:CYS:SG	1.98	1.02
1:C:212:LYS:CD	3:C:1069:HOH:O	2.06	1.02
1:E:173[A]:PRO:HA	3:E:771:HOH:O	1.60	1.00
1:A:125[B]:MET:HB3	1:A:171[B]:CYS:SG	2.00	1.00
1:A:173[A]:PRO:CB	1:C:47[A]:ARG:NH2	2.29	0.95
1:E:125[B]:MET:HE1	3:E:629:HOH:O	1.64	0.95
1:A:125[B]:MET:HE1	3:A:639:HOH:O	1.67	0.92
1:E:4:LEU:N	3:E:501:HOH:O	2.03	0.91
1:D:211:GLN:CD	3:D:502:HOH:O	2.07	0.91
1:C:47[B]:ARG:HH12	1:C:145:ARG:NE	1.70	0.88
1:D:211:GLN:NE2	3:D:502:HOH:O	2.06	0.88
1:C:47[B]:ARG:HH12	1:C:145:ARG:HE	1.22	0.85
1:C:155:ARG:HG3	3:C:786:HOH:O	1.76	0.85
1:D:173[A]:PRO:HA	3:D:812:HOH:O	1.75	0.85
1:E:171[B]:CYS:SG	3:E:537:HOH:O	2.13	0.83
1:B:3:GLU:HG2	3:B:905:HOH:O	1.79	0.83
1:C:47[B]:ARG:NH1	1:C:94:ASP:OD1	2.13	0.82
1:C:47[B]:ARG:NH1	1:C:145:ARG:NE	2.30	0.79
1:D:125[B]:MET:HE2	3:D:631:HOH:O	1.81	0.79
1:D:258:GLU:OE2	3:D:501:HOH:O	2.01	0.78
1:C:125[B]:MET:CG	1:C:171[B]:CYS:SG	2.73	0.76
1:D:337:HIS:HD2	3:D:825:HOH:O	1.68	0.76
1:A:214:LEU:HD13	3:A:604:HOH:O	1.85	0.75
1:A:47[A]:ARG:HH21	1:A:145:ARG:NH2	1.85	0.75
1:C:214:LEU:HD13	3:C:881:HOH:O	1.86	0.75
1:C:250:HIS:HD2	1:C:306:GLU:OE2	1.70	0.74
1:B:211:GLN:HE22	1:B:259:ARG:HH11	1.33	0.74
1:B:47[A]:ARG:NH1	1:E:173[A]:PRO:CB	2.50	0.74
1:D:211:GLN:HE22	1:D:259:ARG:HH11	1.36	0.73
1:D:250:HIS:HD2	1:D:306:GLU:OE2	1.72	0.73
1:C:125[B]:MET:HE2	3:C:849:HOH:O	1.88	0.72
1:D:174[A]:ASP:O	1:D:227:HIS:HD2	1.72	0.72
1:A:250:HIS:HD2	1:A:306:GLU:OE2	1.73	0.72
1:A:50[B]:SER:OG	1:A:52:GLU:OE1	2.07	0.72
1:E:214:LEU:HG	3:E:648:HOH:O	1.90	0.71
1:B:125[B]:MET:HE2	3:B:618:HOH:O	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47[A]:ARG:HH12	1:E:173[A]:PRO:HB2	1.52	0.70
1:B:250:HIS:HD2	1:B:306:GLU:OE2	1.74	0.70
1:E:263:ARG:HG3	3:E:503:HOH:O	1.90	0.70
1:A:125[B]:MET:CB	1:A:171[B]:CYS:SG	2.79	0.70
1:E:250:HIS:HD2	1:E:306:GLU:OE2	1.74	0.69
1:E:125[B]:MET:HG2	3:E:537:HOH:O	1.92	0.69
1:A:173[A]:PRO:HA	3:A:795:HOH:O	1.93	0.68
1:B:263:ARG:HG3	3:B:501:HOH:O	1.93	0.68
1:A:47[A]:ARG:NH2	1:A:145:ARG:NH2	2.41	0.67
1:A:173[A]:PRO:CB	1:C:47[A]:ARG:HH22	2.03	0.66
1:D:172[A]:GLU:HG2	1:D:175:ASN:HB2	1.77	0.65
1:B:172[A]:GLU:O	1:B:172[A]:GLU:HG3	1.96	0.65
1:A:250:HIS:HE1	3:A:534:HOH:O	1.79	0.65
1:A:125[A]:MET:HA	3:A:626:HOH:O	1.97	0.63
1:C:172[A]:GLU:HG2	1:C:175:ASN:HB2	1.80	0.63
1:A:47[A]:ARG:HH21	1:A:145:ARG:HH21	1.47	0.62
1:C:125[B]:MET:HG2	1:C:171[B]:CYS:HG	1.60	0.62
1:B:190:VAL:HG22	1:B:360:LEU:HD23	1.81	0.61
1:D:174[A]:ASP:HA	1:D:228:PRO:HD2	1.83	0.61
1:D:174[A]:ASP:O	1:D:227:HIS:CD2	2.52	0.61
1:C:125[B]:MET:CB	1:C:171[B]:CYS:SG	2.89	0.61
1:A:173[A]:PRO:HB2	1:C:47[A]:ARG:HH21	1.61	0.60
1:E:18:GLN:HE21	1:E:25:THR:H	1.51	0.59
1:E:125[B]:MET:CB	1:E:171[B]:CYS:SG	2.80	0.58
1:E:125[B]:MET:CG	3:E:537:HOH:O	2.49	0.58
1:D:211:GLN:NE2	1:D:259:ARG:HH11	2.01	0.57
1:C:174[A]:ASP:O	1:C:227:HIS:ND1	2.36	0.57
1:E:172[A]:GLU:HG2	1:E:175:ASN:HB2	1.86	0.57
1:B:125[A]:MET:HA	3:B:712:HOH:O	2.04	0.57
1:D:18:GLN:HE21	1:D:25:THR:H	1.53	0.57
1:B:47[A]:ARG:HH12	1:E:173[A]:PRO:CB	2.17	0.56
1:D:211:GLN:HE22	1:D:259:ARG:NH1	2.02	0.56
1:A:18:GLN:HE21	1:A:25:THR:H	1.54	0.56
1:D:125[A]:MET:HA	3:D:703:HOH:O	2.05	0.56
1:E:250:HIS:HE1	3:E:525:HOH:O	1.89	0.56
1:D:174[A]:ASP:OD1	1:D:227:HIS:C	2.45	0.55
1:C:125[B]:MET:HB3	1:C:171[B]:CYS:SG	2.47	0.55
1:A:174[A]:ASP:O	1:A:227:HIS:ND1	2.39	0.54
1:C:18:GLN:HE21	1:C:25:THR:H	1.55	0.54
1:E:174[A]:ASP:O	1:E:227:HIS:ND1	2.41	0.53
1:E:211:GLN:HE22	1:E:259:ARG:HH11	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLN:HE21	1:B:25:THR:H	1.57	0.53
1:D:250:HIS:HE1	3:D:501:HOH:O	1.90	0.53
1:C:144:ARG:HD3	3:C:988:HOH:O	2.08	0.53
1:A:125[B]:MET:CG	3:A:575:HOH:O	2.19	0.52
1:C:174[A]:ASP:OD1	1:C:227:HIS:C	2.48	0.52
1:E:174[B]:ASP:O	1:E:174[B]:ASP:CG	2.48	0.52
1:C:47[B]:ARG:NH2	3:C:701:HOH:O	2.09	0.51
1:D:365:PRO:N	1:D:365:PRO:C	2.56	0.51
1:C:52:GLU:CD	3:C:703:HOH:O	2.48	0.51
1:D:47:ARG:NH1	3:D:504:HOH:O	2.42	0.51
1:E:147:GLU:HG3	3:E:644:HOH:O	2.10	0.51
1:C:266:GLN:HG3	3:C:991:HOH:O	2.10	0.50
1:A:337:HIS:HD2	3:A:775:HOH:O	1.92	0.50
1:C:178[B]:VAL:HG22	1:C:214:LEU:HD23	1.94	0.50
1:E:125[A]:MET:HA	3:E:710:HOH:O	2.11	0.50
1:A:172[A]:GLU:HG2	1:A:175:ASN:HB2	1.93	0.50
1:E:174[A]:ASP:OD1	1:E:227:HIS:C	2.50	0.50
1:A:174[A]:ASP:HA	1:A:228:PRO:HD2	1.94	0.49
1:B:174[A]:ASP:O	1:B:227:HIS:ND1	2.42	0.49
1:C:47[B]:ARG:NH1	1:C:145:ARG:CZ	2.74	0.49
1:B:18:GLN:HE21	1:B:24:VAL:HA	1.77	0.49
1:A:173[A]:PRO:HB2	1:C:47[A]:ARG:CZ	2.34	0.49
1:A:174[A]:ASP:OD1	1:A:227:HIS:C	2.51	0.49
1:B:174[A]:ASP:OD1	1:B:229:GLU:N	2.46	0.48
1:C:18:GLN:HE21	1:C:24:VAL:HA	1.77	0.48
1:A:18:GLN:HE21	1:A:24:VAL:HA	1.79	0.48
1:B:190:VAL:CG2	1:B:360:LEU:HD23	2.44	0.47
1:E:125[B]:MET:N	1:E:171[B]:CYS:SG	2.82	0.47
1:C:172[A]:GLU:HB2	1:C:173[A]:PRO:HD2	1.96	0.47
1:C:219[B]:ARG:CZ	3:C:713:HOH:O	2.61	0.47
1:E:160:GLU:OE2	3:E:502:HOH:O	2.20	0.47
1:E:174[A]:ASP:OD1	1:E:229:GLU:N	2.48	0.47
1:E:61:GLN:HE22	1:E:108:ASP:HB3	1.79	0.47
1:D:174[A]:ASP:CG	1:D:227:HIS:HB3	2.36	0.46
1:E:174[A]:ASP:HA	1:E:228:PRO:HD2	1.97	0.46
1:D:66:TYR:OH	1:D:125[B]:MET:HE3	2.16	0.46
1:E:5:PRO:HG2	3:E:788:HOH:O	2.15	0.46
1:C:22[B]:GLN:HA	1:C:81:ILE:O	2.16	0.46
1:E:18:GLN:HE21	1:E:24:VAL:HA	1.81	0.45
1:B:174[A]:ASP:OD1	1:B:227:HIS:C	2.55	0.45
1:D:174[A]:ASP:OD1	1:D:229:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174[A]:ASP:OD1	1:A:229:GLU:N	2.47	0.45
1:D:250:HIS:CE1	3:D:501:HOH:O	2.67	0.45
1:C:61:GLN:HE22	1:C:108:ASP:HB3	1.81	0.45
1:D:178[B]:VAL:HG23	3:D:695:HOH:O	2.17	0.45
1:E:114:PHE:CE1	1:E:173[B]:PRO:HD2	2.52	0.44
1:C:172[A]:GLU:HB2	1:C:173[A]:PRO:CD	2.47	0.44
1:D:125[B]:MET:CG	3:D:576:HOH:O	2.22	0.44
1:A:174[A]:ASP:CG	1:A:227:HIS:HB3	2.38	0.44
1:C:178[B]:VAL:CG2	1:C:214:LEU:HD23	2.48	0.44
1:B:211:GLN:HE22	1:B:259:ARG:NH1	2.10	0.44
1:B:61:GLN:HE22	1:B:108:ASP:HB3	1.81	0.43
1:A:47[A]:ARG:NH1	3:A:509:HOH:O	2.50	0.43
1:B:47[A]:ARG:HH11	1:B:47[A]:ARG:HD2	1.53	0.43
1:D:61:GLN:HE22	1:D:108:ASP:HB3	1.83	0.43
1:B:152:HIS:HE1	3:B:834:HOH:O	2.01	0.43
1:B:174[A]:ASP:HA	1:B:228:PRO:HD2	2.00	0.43
1:D:18:GLN:HE21	1:D:24:VAL:HA	1.83	0.43
1:C:219[B]:ARG:NE	3:C:713:HOH:O	2.52	0.43
1:C:47[B]:ARG:NH2	1:C:145:ARG:HH21	2.16	0.42
1:A:178[B]:VAL:CG2	1:A:214:LEU:HD23	2.50	0.42
1:A:61:GLN:HE22	1:A:108:ASP:HB3	1.84	0.42
1:C:174[B]:ASP:OD1	1:C:229:GLU:HB2	2.20	0.42
1:E:174[A]:ASP:CG	1:E:227:HIS:HB3	2.40	0.42
3:B:812:HOH:O	1:E:173[A]:PRO:HB3	2.18	0.42
1:C:125[B]:MET:N	1:C:171[B]:CYS:SG	2.80	0.42
1:C:170:VAL:HB	1:C:172[A]:GLU:O	2.19	0.41
1:A:125[B]:MET:CB	3:A:575:HOH:O	2.63	0.41
1:E:171[B]:CYS:HB3	1:E:172[B]:GLU:H	1.73	0.41
1:C:18:GLN:NE2	1:C:25:THR:H	2.18	0.41
1:A:22:GLN:HA	1:A:81:ILE:O	2.21	0.41
1:A:47[A]:ARG:NH2	1:A:145:ARG:HH21	2.09	0.41
1:B:18:GLN:NE2	1:B:25:THR:H	2.18	0.41
1:B:174[A]:ASP:CG	1:B:227:HIS:HB3	2.41	0.41
1:E:18:GLN:NE2	1:E:25:THR:H	2.17	0.41
1:E:47[B]:ARG:HH21	1:E:47[B]:ARG:HD2	1.74	0.41
1:E:250:HIS:CE1	3:E:525:HOH:O	2.70	0.40
1:B:66:TYR:OH	1:B:125[B]:MET:HE3	2.21	0.40
1:C:47[A]:ARG:HH21	1:C:47[A]:ARG:HD2	1.69	0.40
1:A:145:ARG:NH2	3:A:512:HOH:O	2.54	0.40
1:E:363:PRO:HA	1:E:364:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/373 (100%)	358 (96%)	10 (3%)	3 (1%)	19	4
1	B	374/373 (100%)	362 (97%)	8 (2%)	4 (1%)	14	2
1	C	373/373 (100%)	360 (96%)	13 (4%)	0	100	100
1	D	373/373 (100%)	362 (97%)	11 (3%)	0	100	100
1	E	369/373 (99%)	357 (97%)	11 (3%)	1 (0%)	41	18
All	All	1860/1865 (100%)	1799 (97%)	53 (3%)	8 (0%)	41	13

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174[A]	ASP
1	B	174[B]	ASP
1	A	171[A]	CYS
1	A	171[B]	CYS
1	B	173[A]	PRO
1	B	173[B]	PRO
1	A	212	LYS
1	E	212	LYS

### 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	303/302 (100%)	299 (99%)	4 (1%)	69 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	304/302 (101%)	300 (99%)	4 (1%)	69	40
1	C	304/302 (101%)	301 (99%)	3 (1%)	76	52
1	D	302/302 (100%)	299 (99%)	3 (1%)	76	52
1	E	301/302 (100%)	298 (99%)	3 (1%)	76	52
All	All	1514/1510 (100%)	1497 (99%)	17 (1%)	73	48

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	240	TYR
1	A	254	PRO
1	A	360	LEU
1	B	171[A]	CYS
1	B	171[B]	CYS
1	B	228	PRO
1	B	240	TYR
1	C	4	LEU
1	C	204	ARG
1	C	240	TYR
1	D	229	GLU
1	D	240	TYR
1	D	363	PRO
1	E	61	GLN
1	E	240	TYR
1	E	274	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	61	GLN
1	A	250	HIS
1	B	18	GLN
1	B	61	GLN
1	B	152	HIS
1	B	211	GLN
1	B	250	HIS
1	C	18	GLN
1	C	61	GLN

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Mol	Chain	Res	Type
1	C	152	HIS
1	C	211	GLN
1	C	250	HIS
1	D	18	GLN
1	D	61	GLN
1	D	211	GLN
1	D	227	HIS
1	D	250	HIS
1	D	310	GLN
1	E	18	GLN
1	E	61	GLN
1	E	211	GLN
1	E	250	HIS
1	E	310	GLN

### 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](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	A	402	-	3,3,3	0.18	0	2,2,2	0.46	0
2	EDO	C	402	-	3,3,3	0.46	0	2,2,2	0.33	0
2	EDO	B	401	-	3,3,3	0.58	0	2,2,2	0.60	0
2	EDO	C	401	-	3,3,3	0.50	0	2,2,2	0.26	0
2	EDO	E	401	-	3,3,3	0.57	0	2,2,2	0.59	0
2	EDO	A	401	-	3,3,3	0.39	0	2,2,2	0.40	0
2	EDO	B	403	-	3,3,3	0.45	0	2,2,2	1.03	0
2	EDO	D	401	-	3,3,3	0.42	0	2,2,2	0.22	0
2	EDO	B	402	-	3,3,3	0.15	0	2,2,2	0.47	0
2	EDO	B	404	-	3,3,3	0.27	0	2,2,2	0.29	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	402	-	-	0/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-
2	EDO	C	401	-	-	0/1/1/1	-
2	EDO	E	401	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	B	403	-	-	0/1/1/1	-
2	EDO	D	401	-	-	0/1/1/1	-
2	EDO	B	402	-	-	0/1/1/1	-
2	EDO	B	404	-	-	0/1/1/1	-

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.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	171[A]:CYS	C	172[A]:GLU	N	1.19

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	363/373 (97%)	-0.03	5 (1%) 75 76	13, 18, 31, 47	0
1	B	368/373 (98%)	-0.05	4 (1%) 80 82	12, 16, 28, 50	0
1	C	364/373 (97%)	-0.01	4 (1%) 80 82	12, 18, 30, 46	0
1	D	364/373 (97%)	0.00	4 (1%) 80 82	12, 17, 28, 53	0
1	E	363/373 (97%)	-0.03	6 (1%) 70 70	13, 19, 30, 59	0
All	All	1822/1865 (97%)	-0.02	23 (1%) 77 78	12, 18, 30, 59	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171[A]	CYS	6.1
1	A	171[A]	CYS	4.2
1	C	173[A]	PRO	3.9
1	E	4	LEU	3.9
1	C	171[A]	CYS	3.8
1	E	366	ALA	3.3
1	B	367	ALA	3.3
1	E	171[A]	CYS	3.3
1	E	7	GLY	3.0
1	D	4	LEU	3.0
1	A	6	PRO	2.8
1	B	0	ALA	2.8
1	A	4	LEU	2.7
1	D	125[A]	MET	2.6
1	C	174[A]	ASP	2.6
1	D	213	ASP	2.5
1	B	172[A]	GLU	2.5
1	A	173[A]	PRO	2.2
1	A	125[A]	MET	2.2
1	D	171[A]	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	6	PRO	2.1
1	E	213	ASP	2.1
1	C	360	LEU	2.1

## 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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	EDO	B	404	4/4	0.86	0.29	35,36,38,38	0
2	EDO	C	401	4/4	0.90	0.13	23,24,24,24	0
2	EDO	A	401	4/4	0.92	0.09	20,22,23,26	0
2	EDO	A	402	4/4	0.92	0.14	30,33,34,35	0
2	EDO	D	401	4/4	0.92	0.10	21,23,23,24	0
2	EDO	C	402	4/4	0.93	0.10	29,30,34,38	0
2	EDO	B	402	4/4	0.94	0.11	24,27,35,37	0
2	EDO	E	401	4/4	0.94	0.08	22,23,23,23	0
2	EDO	B	403	4/4	0.95	0.13	24,28,31,37	0
2	EDO	B	401	4/4	0.95	0.10	20,22,22,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.