



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:14 pm BST

PDB ID : 2B3X  
Title : Structure of an orthorhombic crystal form of human cytosolic aconitase (IRP1)  
Authors : Dupuy, J.; Fontecilla-Camps, J.C.; Volbeda, A.  
Deposited on : 2005-09-22  
Resolution : 2.54 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.

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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	:	2.11
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)	:	2.11

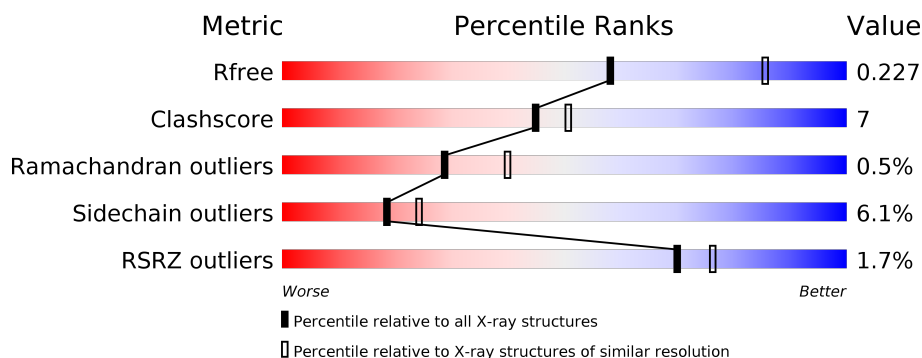
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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  $\geq 3$ , 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	888	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7109 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.

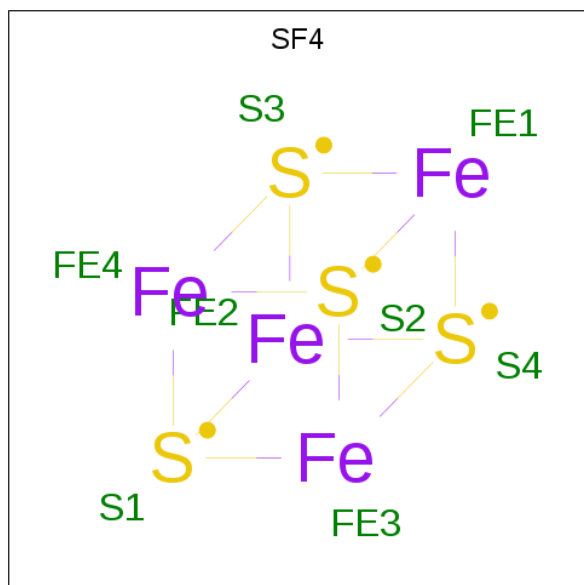
- Molecule 1 is a protein called Iron-responsive element binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	888	Total	C	N	O	S	47	0	0
			6928	4431	1183	1285	29			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 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
4	A	1	Total	C	O	0	0
			4	2	2		

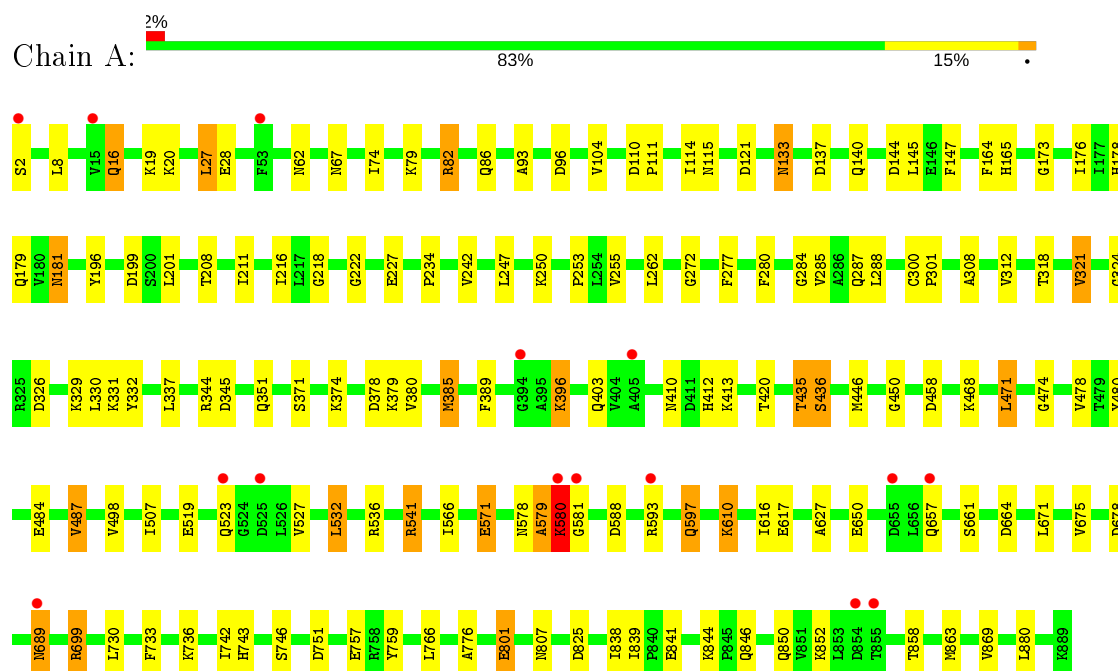
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	168	Total	O	0	0
			168	168		

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

These plots are drawn for all protein, RNA and DNA 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: Iron-responsive element binding protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.35Å 103.31Å 225.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.23 – 2.54 47.35 – 2.54	Depositor EDS
% Data completeness (in resolution range)	96.9 (113.23-2.54) 96.9 (47.35-2.54)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.180 , 0.225 0.184 , 0.227	Depositor DCC
$R_{free}$ test set	1435 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 29.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: ZN, SF4, 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	0.67	13/7089 (0.2%)	0.83	19/9626 (0.2%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	536	ARG	NE-CZ	-20.36	1.06	1.33
1	A	541	ARG	CG-CD	15.18	1.89	1.51
1	A	825	ASP	CB-CG	-12.50	1.25	1.51
1	A	579	ALA	C-N	-11.74	1.07	1.34
1	A	757	GLU	CB-CG	-11.50	1.30	1.52
1	A	326	ASP	CB-CG	-9.20	1.32	1.51
1	A	841	GLU	CG-CD	-7.95	1.40	1.51
1	A	650	GLU	CG-CD	-7.66	1.40	1.51
1	A	801	GLU	CD-OE2	7.28	1.33	1.25
1	A	801	GLU	CG-CD	6.89	1.62	1.51
1	A	28	GLU	CB-CG	-5.73	1.41	1.52
1	A	571	GLU	CG-CD	5.58	1.60	1.51
1	A	579	ALA	N-CA	-5.15	1.36	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	ARG	NE-CZ-NH2	-23.81	108.39	120.30
1	A	536	ARG	NE-CZ-NH1	21.33	130.96	120.30
1	A	326	ASP	CB-CG-OD2	11.54	128.69	118.30
1	A	326	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	A	825	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	458	ASP	CB-CG-OD2	5.96	123.67	118.30
1	A	541	ARG	CG-CD-NE	5.83	124.03	111.80
1	A	536	ARG	CD-NE-CZ	-5.82	115.45	123.60
1	A	378	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	841	GLU	CG-CD-OE1	5.51	129.33	118.30
1	A	588	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	841	GLU	CG-CD-OE2	-5.21	107.89	118.30
1	A	121	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	664	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	96	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	751	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	144	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	532	LEU	CA-CB-CG	5.06	126.95	115.30
1	A	541	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	579	ALA	Mainchain

## 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	6928	0	6919	90	0
2	A	1	0	0	0	0
3	A	8	0	0	0	0
4	A	4	0	6	1	0
5	A	168	0	0	15	0
All	All	7109	0	6925	90	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 7.

All (90) 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:345:ASP:H	1:A:351:GLN:HE22	1.13	0.96
1:A:396:LYS:HE3	1:A:396:LYS:H	1.27	0.96
1:A:519:GLU:O	1:A:523:GLN:HG2	1.69	0.93
1:A:82:ARG:HH22	1:A:181:ASN:HD21	0.99	0.91
1:A:82:ARG:HH22	1:A:181:ASN:ND2	1.68	0.90
1:A:287:GLN:HB3	5:A:1148:HOH:O	1.80	0.82
1:A:743:HIS:HE1	5:A:1151:HOH:O	1.61	0.82
1:A:420:THR:CG2	5:A:1170:HOH:O	2.28	0.80
1:A:420:THR:HG22	5:A:1170:HOH:O	1.83	0.79
1:A:222:GLY:HA3	1:A:807:ASN:HD21	1.53	0.72
1:A:396:LYS:HE3	1:A:396:LYS:N	2.06	0.69
1:A:580:LYS:HD2	1:A:581:GLY:N	2.07	0.69
1:A:699:ARG:HH21	1:A:699:ARG:CG	2.06	0.69
1:A:201:LEU:HD21	1:A:211:ILE:HG21	1.74	0.68
1:A:396:LYS:CE	1:A:396:LYS:H	2.04	0.65
1:A:420:THR:HG21	5:A:1170:HOH:O	1.96	0.64
1:A:345:ASP:H	1:A:351:GLN:NE2	1.91	0.63
1:A:743:HIS:CE1	5:A:1151:HOH:O	2.43	0.62
1:A:93:ALA:HA	1:A:227:GLU:OE2	2.00	0.60
1:A:82:ARG:HD3	1:A:199:ASP:OD1	2.02	0.60
1:A:345:ASP:N	1:A:351:GLN:HE22	1.93	0.59
1:A:115:ASN:ND2	1:A:165:HIS:H	2.01	0.59
1:A:699:ARG:HG3	1:A:699:ARG:HH21	1.68	0.58
1:A:179:GLN:OE1	1:A:474:GLY:HA3	2.03	0.56
1:A:104:VAL:HG21	1:A:114:ILE:CD1	2.37	0.54
1:A:201:LEU:O	1:A:218:GLY:HA2	2.06	0.54
1:A:253:PRO:HA	1:A:593:ARG:HH21	1.72	0.54
1:A:253:PRO:HA	1:A:593:ARG:HE	1.74	0.53
1:A:689:ASN:H	1:A:689:ASN:HD22	1.56	0.53
1:A:324:GLY:O	1:A:610:LYS:HE3	2.10	0.52
1:A:743:HIS:HD2	1:A:746:SER:OG	1.93	0.50
1:A:435:THR:O	1:A:436:SER:HB3	2.11	0.50
1:A:82:ARG:NH2	1:A:181:ASN:ND2	2.50	0.49
1:A:593:ARG:O	1:A:597:GLN:HB2	2.12	0.49
1:A:227:GLU:OE1	1:A:880:LEU:HD11	2.13	0.49
1:A:255:VAL:O	1:A:593:ARG:HD3	2.13	0.48
1:A:468:LYS:HE3	5:A:1144:HOH:O	2.11	0.48
1:A:446:MET:HE1	1:A:471:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:THR:HG22	5:A:1005:HOH:O	2.13	0.48
1:A:284:GLY:O	1:A:287:GLN:HG2	2.13	0.48
1:A:616:ILE:HD12	5:A:1142:HOH:O	2.13	0.48
1:A:776:ALA:HA	1:A:801:GLU:HG3	1.96	0.48
1:A:838:ILE:HD11	1:A:852:LYS:HD3	1.96	0.48
1:A:519:GLU:O	1:A:523:GLN:CG	2.53	0.48
1:A:8:LEU:HD11	1:A:27:LEU:HD13	1.96	0.47
1:A:344:ARG:HH11	1:A:351:GLN:HE21	1.61	0.47
1:A:247:LEU:HD12	1:A:285:VAL:HG22	1.97	0.46
1:A:133:ASN:HD21	4:A:1002:EDO:H12	1.81	0.46
1:A:137:ASP:HB3	5:A:1103:HOH:O	2.16	0.45
1:A:838:ILE:HD13	1:A:850:GLN:HG3	1.98	0.45
1:A:300:CYS:N	1:A:301:PRO:HD2	2.31	0.45
1:A:671:LEU:HB3	1:A:675:VAL:HG21	1.97	0.45
1:A:318:THR:HA	1:A:321:VAL:HG13	1.98	0.45
1:A:62:ASN:HB3	1:A:74:ILE:HD11	1.97	0.45
1:A:20:LYS:HE2	5:A:1168:HOH:O	2.17	0.45
1:A:435:THR:O	1:A:436:SER:CB	2.64	0.45
1:A:389:PHE:CG	1:A:566:ILE:HD11	2.52	0.45
1:A:699:ARG:NH2	1:A:699:ARG:CG	2.69	0.45
1:A:699:ARG:NH2	1:A:699:ARG:HG2	2.31	0.44
1:A:759:TYR:CG	1:A:766:LEU:HD21	2.52	0.44
1:A:627:ALA:N	5:A:1157:HOH:O	2.39	0.44
1:A:16:GLN:HB3	1:A:16:GLN:HE21	1.65	0.44
1:A:523:GLN:OE1	1:A:523:GLN:HA	2.17	0.44
1:A:173:GLY:HA2	5:A:1016:HOH:O	2.16	0.43
1:A:280:PHE:HE1	1:A:308:ALA:HB1	1.84	0.43
1:A:374:LYS:HE2	5:A:1167:HOH:O	2.18	0.43
1:A:410:ASN:O	1:A:412:HIS:HD2	2.01	0.43
1:A:616:ILE:HG23	1:A:617:GLU:HG3	2.00	0.43
1:A:689:ASN:N	1:A:689:ASN:HD22	2.15	0.43
1:A:329:LYS:HG3	1:A:332:TYR:OH	2.18	0.43
1:A:176:ILE:HG13	1:A:474:GLY:HA2	2.00	0.42
1:A:329:LYS:HA	1:A:332:TYR:CE2	2.54	0.42
1:A:471:LEU:HD13	1:A:498:VAL:HG22	2.02	0.42
1:A:661:SER:HA	1:A:839:ILE:HD12	2.02	0.42
1:A:110:ASP:HA	1:A:111:PRO:HD3	1.90	0.42
1:A:82:ARG:NH2	1:A:181:ASN:HD21	1.85	0.42
1:A:733:PHE:HB3	1:A:742:ILE:HD12	2.02	0.42
1:A:385:MET:HE2	1:A:385:MET:CA	2.49	0.41
1:A:79:LYS:HG3	1:A:234:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LYS:HB3	1:A:196:TYR:CE2	2.54	0.41
1:A:242:VAL:HG22	1:A:277:PHE:HB2	2.01	0.41
1:A:385:MET:HE2	1:A:385:MET:HA	2.02	0.41
1:A:199:ASP:HB3	1:A:216:ILE:HG12	2.02	0.41
1:A:178:HIS:CE1	1:A:208:THR:HA	2.55	0.41
1:A:287:GLN:CB	5:A:1148:HOH:O	2.54	0.41
1:A:450:GLY:HA3	1:A:487:VAL:HG11	2.03	0.41
1:A:846:GLN:HA	1:A:863:MET:O	2.20	0.41
1:A:312:VAL:HG11	1:A:337:LEU:HD13	2.03	0.41
1:A:115:ASN:ND2	1:A:164:PHE:HA	2.36	0.40
1:A:331:LYS:HD3	1:A:331:LYS:HA	1.94	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	886/888 (100%)	857 (97%)	25 (3%)	4 (0%)	29	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	580	LYS
1	A	403	GLN
1	A	436	SER
1	A	272	GLY

### 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	751/751 (100%)	705 (94%)	46 (6%)	18	24

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	16	GLN
1	A	27	LEU
1	A	67	ASN
1	A	82	ARG
1	A	86	GLN
1	A	133	ASN
1	A	140	GLN
1	A	145	LEU
1	A	147	PHE
1	A	181	ASN
1	A	250	LYS
1	A	262	LEU
1	A	288	LEU
1	A	321	VAL
1	A	330	LEU
1	A	371	SER
1	A	379	LYS
1	A	380	VAL
1	A	385	MET
1	A	396	LYS
1	A	413	LYS
1	A	435	THR
1	A	471	LEU
1	A	478	VAL
1	A	480	TYR
1	A	484	GLU
1	A	487	VAL
1	A	507	ILE
1	A	527	VAL
1	A	532	LEU
1	A	541	ARG
1	A	571	GLU
1	A	578	ASN

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Mol	Chain	Res	Type
1	A	580	LYS
1	A	597	GLN
1	A	610	LYS
1	A	657	GLN
1	A	678	ASP
1	A	689	ASN
1	A	699	ARG
1	A	730	LEU
1	A	736	LYS
1	A	844	LYS
1	A	858	THR
1	A	869	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	62	ASN
1	A	65	HIS
1	A	115	ASN
1	A	133	ASN
1	A	181	ASN
1	A	233	GLN
1	A	351	GLN
1	A	403	GLN
1	A	412	HIS
1	A	439	ASN
1	A	509	ASN
1	A	545	ASN
1	A	602	GLN
1	A	689	ASN
1	A	698	ASN
1	A	743	HIS
1	A	807	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z  > 2$
3	SF4	A	1000	1,5	0,12,12	0.00	-	-		
4	EDO	A	1002	-	3,3,3	0.60	0	2,2,2	0.04	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
3	SF4	A	1000	1,5	-	-	0/6/5/5
4	EDO	A	1002	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	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	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	579:ALA	C	580:LYS	N	1.07

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	888/888 (100%)	-0.01	15 (1%) 70 76	18, 31, 47, 68	59 (6%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	580	LYS	4.4
1	A	53	PHE	3.1
1	A	689	ASN	3.0
1	A	655	ASP	2.8
1	A	593	ARG	2.7
1	A	405	ALA	2.6
1	A	2	SER	2.5
1	A	523	GLN	2.4
1	A	581	GLY	2.3
1	A	854	ASP	2.3
1	A	394	GLY	2.3
1	A	15	VAL	2.3
1	A	525	ASP	2.1
1	A	855	THR	2.1
1	A	657	GLN	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. 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( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	1002	4/4	0.88	0.17	30,31,31,32	0
2	ZN	A	1001	1/1	0.98	0.05	50,50,50,50	0
3	SF4	A	1000	8/8	0.99	0.10	20,22,23,24	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.