



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 05:07 pm GMT

PDB ID : 3RNF
Title : Structure of the Toluene/o-Xylene Monooxygenase Hydroxylase T201S/V271A Double Mutant
Authors : Gucinski, G.; Song, W.J.; Lippard, S.J.; Sazinsky, M.H.
Deposited on : 2011-04-22
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

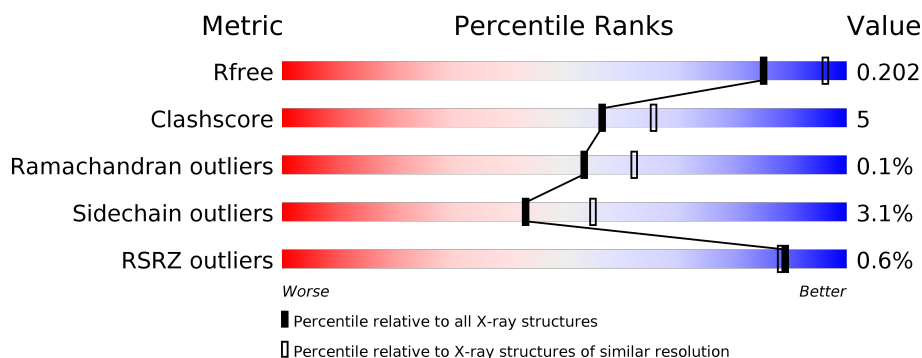
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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	498	 87% 11% ..
2	B	330	 83% 13% . .
3	C	86	 79% 17% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7923 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 Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			4015	2562	674	753	26			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	SER	THR	ENGINEERED MUTATION	UNP Q6IV66
A	271	ALA	VAL	ENGINEERED MUTATION	UNP Q6IV66
A	445	LYS	GLU	ENGINEERED MUTATION	UNP Q6IV66

- Molecule 2 is a protein called Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	323	Total	C	N	O	S	0	0	0
			2649	1680	468	491	10			

- Molecule 3 is a protein called Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	85	Total	C	N	O	S	0	0	0
			689	432	123	129	5			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

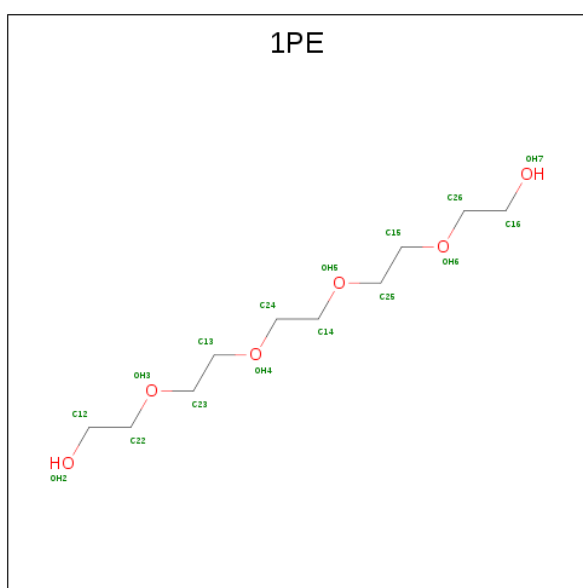


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Fe	0	0
			2	2		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	286	Total	O	0	0
			286	286		
7	B	222	Total	O	0	0
			222	222		
7	C	40	Total	O	0	0
			40	40		

- Molecule 1: Toluene o-xylene monooxygenase component



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.34Å 183.34Å 68.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.84 – 2.20 45.84 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.84-2.20) 99.6 (45.84-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.71 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.154 , 0.200 0.157 , 0.202	Depositor DCC
R_{free} test set	3372 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7923	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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, 0.333 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: 1PE, EDO, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.11	1/4139 (0.0%)	0.88	7/5624 (0.1%)
2	B	1.13	3/2721 (0.1%)	0.87	1/3699 (0.0%)
3	C	1.07	1/703 (0.1%)	0.92	2/952 (0.2%)
All	All	1.11	5/7563 (0.1%)	0.88	10/10275 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	GLU	CB-CG	5.56	1.62	1.52
2	B	290	ALA	CA-CB	5.32	1.63	1.52
2	B	262	GLU	CG-CD	5.24	1.59	1.51
3	C	32	GLU	CG-CD	5.14	1.59	1.51
2	B	98	GLN	CB-CG	5.05	1.66	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	107	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	A	84	ARG	NE-CZ-NH2	-5.60	117.50	120.30
3	C	12	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	252	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	48	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	6	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	450	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	A	264	ARG	NE-CZ-NH1	5.03	122.81	120.30
3	C	13	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	443	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4015	0	3767	41	0
2	B	2649	0	2548	37	0
3	C	689	0	678	14	0
4	A	4	0	5	0	0
5	A	2	0	0	0	0
6	A	16	0	22	1	0
7	A	286	0	0	4	0
7	B	222	0	0	2	0
7	C	40	0	0	1	0
All	All	7923	0	7020	78	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 5.

All (78) 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:427:HIS:HE1	3:C:76:THR:HG23	1.24	0.98
1:A:427:HIS:HE1	3:C:76:THR:CG2	1.75	0.98
3:C:75:PRO:O	3:C:76:THR:HB	1.64	0.97
1:A:427:HIS:CE1	3:C:76:THR:HG23	2.02	0.94
2:B:262:GLU:HG2	7:B:346:HOH:O	1.77	0.83
1:A:416:ASP:OD2	1:A:427:HIS:HD2	1.61	0.81
1:A:19:THR:O	2:B:203:ARG:NH2	2.14	0.81
1:A:139:GLN:HE22	2:B:83:TYR:H	1.31	0.78
1:A:445:LYS:HD3	7:A:729:HOH:O	1.83	0.76
1:A:427:HIS:CE1	3:C:76:THR:CG2	2.66	0.69
1:A:113:ARG:HH11	2:B:144:GLN:HE21	1.39	0.69
2:B:168:HIS:HD2	2:B:257:GLN:HE21	1.41	0.69
1:A:7:GLU:H	1:A:7:GLU:CD	1.96	0.67
2:B:162:HIS:HE1	2:B:227:LYS:HZ2	1.43	0.67
1:A:396:ILE:HG13	1:A:451:VAL:HG23	1.76	0.66
7:A:614:HOH:O	2:B:36:HIS:HD2	1.78	0.66
2:B:81:LEU:HD11	2:B:263:ARG:HD2	1.79	0.65
1:A:154:LYS:HG2	1:A:343:TRP:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:PRO:O	3:C:76:THR:CB	2.44	0.64
3:C:11:GLU:HG2	3:C:12:ARG:HG3	1.79	0.64
1:A:305:GLN:HA	1:A:305:GLN:HE21	1.63	0.62
1:A:416:ASP:H	3:C:56:HIS:CE1	2.19	0.61
1:A:92:THR:HG23	1:A:276:ILE:HD13	1.83	0.61
1:A:281:THR:HG21	7:A:747:HOH:O	2.00	0.60
1:A:398:ASN:HD22	1:A:427:HIS:H	1.48	0.59
2:B:305:SER:HB3	2:B:314:ILE:HD11	1.85	0.59
1:A:281:THR:HG22	7:A:706:HOH:O	2.03	0.59
1:A:425:LEU:HD23	3:C:76:THR:HG22	1.84	0.59
1:A:5:LYS:HB3	1:A:7:GLU:OE1	2.02	0.59
2:B:168:HIS:CD2	2:B:257:GLN:HE21	2.20	0.57
2:B:162:HIS:HE1	2:B:227:LYS:NZ	2.01	0.57
1:A:152:SER:HA	2:B:11:PRO:HG3	1.86	0.56
1:A:314:PRO:HD2	1:A:317:TRP:CE3	2.41	0.56
2:B:276:LEU:HD22	2:B:282:ARG:HB2	1.88	0.56
3:C:56:HIS:HD2	3:C:80:ASP:OD1	1.88	0.55
2:B:111:GLN:H	2:B:111:GLN:NE2	2.05	0.54
1:A:139:GLN:NE2	2:B:83:TYR:H	2.05	0.54
1:A:416:ASP:OD2	1:A:427:HIS:CD2	2.52	0.52
1:A:2:SER:N	2:B:105:ASN:HD22	2.07	0.52
1:A:153:ARG:O	1:A:156:ASP:N	2.34	0.52
2:B:8:ALA:N	7:B:494:HOH:O	2.43	0.51
2:B:327:MET:HA	2:B:327:MET:HE2	1.92	0.51
1:A:221:ALA:O	1:A:225:SER:HB3	2.10	0.51
2:B:326:GLN:HG3	2:B:327:MET:HE3	1.93	0.51
1:A:418:GLN:HE22	3:C:78:THR:H	1.57	0.50
1:A:338:TRP:CD1	1:A:390:PRO:HG3	2.47	0.50
1:A:127:ALA:HB2	1:A:237:GLN:HE22	1.77	0.49
2:B:33:THR:HB	2:B:34:ASN:HD22	1.78	0.49
2:B:111:GLN:H	2:B:111:GLN:HE21	1.60	0.48
3:C:48:GLU:HB2	7:C:175:HOH:O	2.12	0.48
3:C:55:ARG:HD2	3:C:58:ASP:OD1	2.14	0.48
2:B:326:GLN:HE21	2:B:327:MET:CE	2.27	0.47
2:B:24:ARG:HA	2:B:25:PRO:HD3	1.80	0.47
1:A:391:GLU:HA	1:A:464:LEU:HD11	1.96	0.46
2:B:36:HIS:HE1	2:B:152:THR:OG1	1.97	0.46
2:B:184:GLY:HA3	2:B:188:ARG:HD3	1.97	0.46
1:A:153:ARG:O	1:A:154:LYS:C	2.54	0.46
1:A:276:ILE:O	1:A:281:THR:HG23	2.16	0.46
2:B:154:CYS:HB3	2:B:267:TRP:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:GLY:HA3	2:B:299:ALA:HA	1.97	0.46
2:B:287:LYS:HB2	2:B:287:LYS:HZ2	1.81	0.46
2:B:249:LEU:HD23	2:B:249:LEU:C	2.37	0.45
2:B:94:GLU:OE1	2:B:168:HIS:HE1	1.99	0.45
2:B:143:HIS:CD2	2:B:143:HIS:C	2.91	0.44
2:B:154:CYS:HB3	2:B:267:TRP:CD2	2.53	0.44
2:B:172:ARG:CZ	2:B:249:LEU:HD13	2.48	0.43
1:A:460:GLN:HA	1:A:461:PRO:C	2.39	0.43
2:B:17:HIS:HE1	2:B:33:THR:OG1	2.00	0.43
3:C:2:ALA:HA	3:C:23:THR:OG1	2.19	0.42
1:A:405:ALA:O	1:A:406:HIS:HB2	2.20	0.42
1:A:113:ARG:HD3	2:B:144:GLN:NE2	2.35	0.41
1:A:107:ALA:O	1:A:110:ALA:HB3	2.21	0.41
1:A:394:PRO:CG	6:A:502:1PE:H222	2.50	0.41
1:A:107:ALA:O	1:A:110:ALA:N	2.54	0.41
1:A:49:GLU:O	1:A:49:GLU:HG2	2.21	0.41
2:B:21:ASN:O	2:B:22:ARG:CB	2.68	0.41
2:B:326:GLN:HG3	2:B:327:MET:CE	2.51	0.41
1:A:175:PHE:CE1	1:A:179:MET:HG3	2.56	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	489/498 (98%)	472 (96%)	16 (3%)	1 (0%)	49	57
2	B	321/330 (97%)	315 (98%)	6 (2%)	0	100	100
3	C	83/86 (96%)	78 (94%)	5 (6%)	0	100	100
All	All	893/914 (98%)	865 (97%)	27 (3%)	1 (0%)	53	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	PRO

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	416/421 (99%)	407 (98%)	9 (2%)	55	68
2	B	275/282 (98%)	264 (96%)	11 (4%)	34	43
3	C	78/79 (99%)	74 (95%)	4 (5%)	26	31
All	All	769/782 (98%)	745 (97%)	24 (3%)	43	55

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	78	ARG
1	A	100	ILE
1	A	206	LEU
1	A	280	TYR
1	A	283	LEU
1	A	304	ARG
1	A	305	GLN
1	A	396	ILE
2	B	22	ARG
2	B	23	ARG
2	B	24	ARG
2	B	45	PRO
2	B	89	LEU
2	B	107	ARG
2	B	111	GLN
2	B	140	VAL
2	B	188	ARG
2	B	248	THR
2	B	283	GLU
3	C	50	ILE
3	C	66	MET

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Mol	Chain	Res	Type
3	C	69	SER
3	C	76	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	139	GLN
1	A	237	GLN
1	A	305	GLN
1	A	379	ASN
1	A	398	ASN
1	A	418	GLN
1	A	427	HIS
2	B	17	HIS
2	B	34	ASN
2	B	36	HIS
2	B	80	GLN
2	B	111	GLN
2	B	144	GLN
2	B	153	ASN
2	B	162	HIS
2	B	168	HIS
2	B	326	GLN
3	C	56	HIS

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 4 ligands modelled in this entry, 2 are 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$
4	EDO	A	499	5	3,3,3	0.51	0	2,2,2	0.34	0
6	1PE	A	502	-	15,15,15	0.60	0	14,14,14	1.22	1 (7%)

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	EDO	A	499	5	-	0/1/1/1	0/0/0/0
6	1PE	A	502	-	-	0/13/13/13	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	A	502	1PE	OH5-C14-C24	-2.31	99.70	110.37

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
6	A	502	1PE	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 [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, 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	491/498 (98%)	-0.65	2 (0%) 92 91	13, 22, 36, 53	0
2	B	323/330 (97%)	-0.72	3 (0%) 84 83	13, 20, 38, 70	0
3	C	85/86 (98%)	-0.81	0 100 100	18, 26, 37, 52	0
All	All	899/914 (98%)	-0.69	5 (0%) 89 88	13, 22, 37, 70	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	22	ARG	5.1
2	B	23	ARG	4.2
2	B	21	ASN	3.8
1	A	107	ALA	2.3
1	A	304	ARG	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 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, 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	B-factors(\AA^2)	Q<0.9
6	1PE	A	502	16/16	0.93	0.13	26,36,45,51	0
4	EDO	A	499	4/4	0.96	0.26	22,29,32,38	0
5	FE	A	501	1/1	1.00	0.10	21,21,21,21	0
5	FE	A	500	1/1	1.00	0.09	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.