



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:28 AM UTC

PDB ID : 5AK3 / pdb_00005ak3
Title : ligand complex structure of soluble epoxide hydrolase
Authors : Oster, L.; Tapani, S.; Xue, Y.; Kack, H.
Deposited on : 2015-03-02
Resolution : 2.28 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

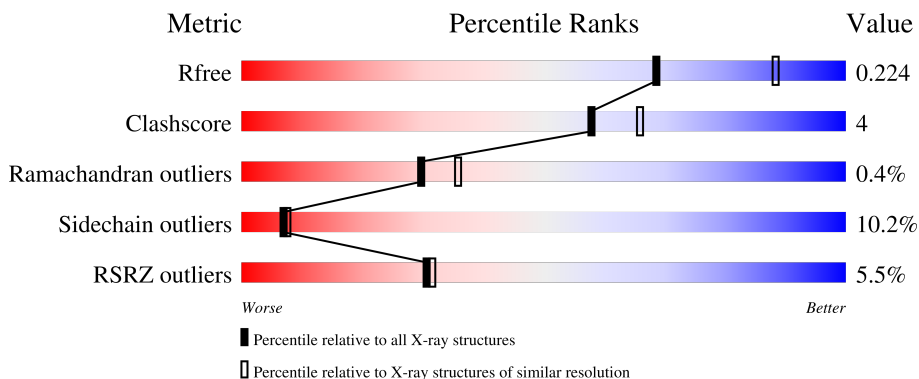
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	549	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMS	A	1552	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4536 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 BIFUNCTIONAL EPOXIDE HYDROLASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	547	4340	2781	731	790	38	0	2	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P34913

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



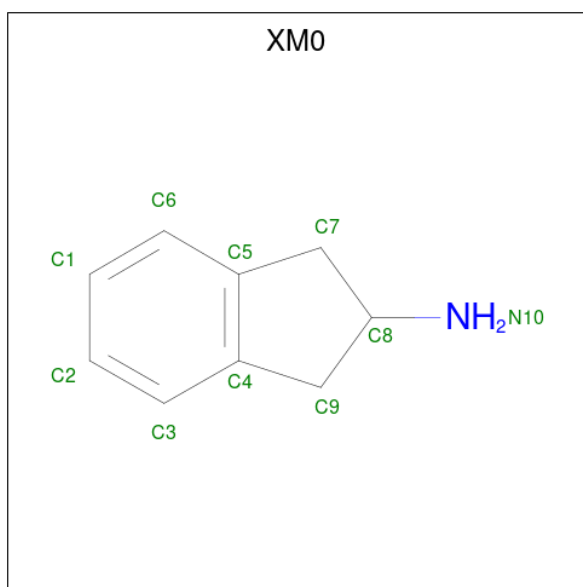
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 4 is INDAN-2-AMINE (CCD ID: XM0) (formula: C₉H₁₁N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			10	9	1		

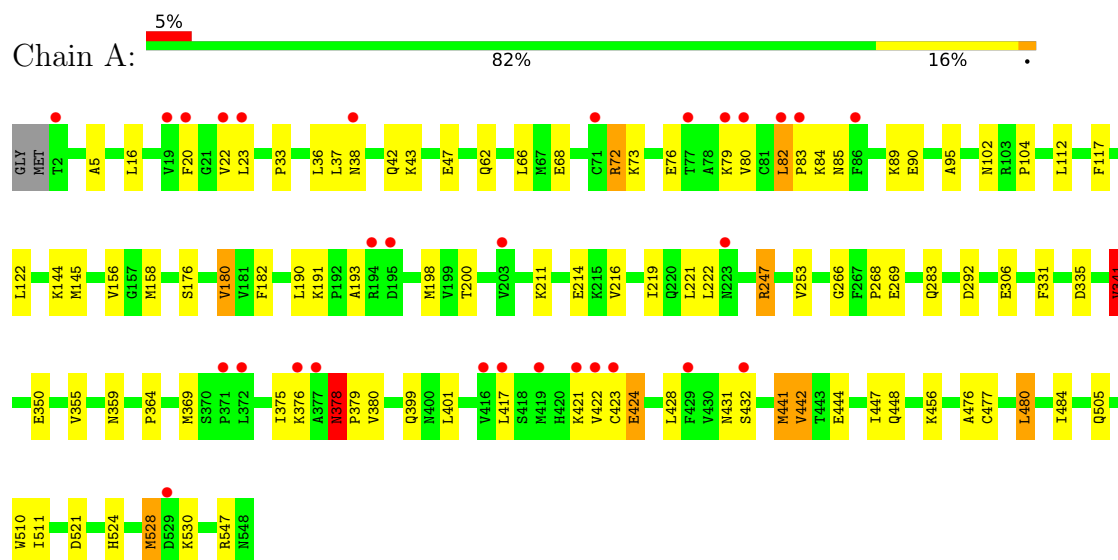
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	164	Total 164	O 164	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: BIFUNCTIONAL EPOXIDE HYDROLASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.97Å 92.97Å 245.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.29 – 2.28 67.29 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.1 (67.29-2.28) 98.1 (67.29-2.28)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.27Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.196 , 0.218 0.201 , 0.224	Depositor DCC
R_{free} test set	1470 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4536	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: DMS, XM0, SO4

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	0.82	2/4445 (0.0%)	1.34	15/6022 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	MET	SD-CE	-6.33	1.63	1.79
1	A	547	ARG	C-N	-5.40	1.25	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	LYS	N-CA-C	6.95	118.85	111.28
1	A	269	GLU	N-CA-C	6.73	118.78	109.29
1	A	505	GLN	N-CA-C	6.73	119.47	111.33
1	A	292	ASP	N-CA-C	-6.37	97.31	108.20
1	A	180	VAL	N-CA-C	6.29	116.92	108.11
1	A	378	ASN	N-CA-C	5.60	119.40	107.91
1	A	444	GLU	CA-C-N	5.34	127.43	120.28
1	A	444	GLU	C-N-CA	5.34	127.43	120.28
1	A	90	GLU	CB-CG-CD	5.22	121.47	112.60
1	A	83	PRO	CA-C-N	5.18	131.44	121.54
1	A	83	PRO	C-N-CA	5.18	131.44	121.54
1	A	37	LEU	CA-C-N	5.11	127.12	120.28
1	A	37	LEU	C-N-CA	5.11	127.12	120.28
1	A	182	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	341	VAL	CB-CA-C	5.08	119.00	112.14

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	4340	0	4345	39	0
2	A	10	0	0	0	0
3	A	12	0	18	0	0
4	A	10	0	11	1	0
5	A	164	0	0	1	0
All	All	4536	0	4374	39	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 4.

All (39) 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:331:PHE:HB3	1:A:341:VAL:HG22	1.54	0.89
1:A:247:ARG:HH11	1:A:247:ARG:HG2	1.40	0.86
1:A:378:ASN:HD22	1:A:380:VAL:HG22	1.41	0.83
1:A:364:PRO:HG2	1:A:510:TRP:CE2	2.19	0.77
1:A:341:VAL:HG13	1:A:355:VAL:HG23	1.71	0.72
1:A:190:LEU:HD22	1:A:200:THR:HB	1.74	0.69
1:A:441:MET:HE3	1:A:528:MET:HE2	1.75	0.68
1:A:33:PRO:HG2	1:A:80:VAL:HG21	1.75	0.68
1:A:72:ARG:HH11	1:A:72:ARG:HG3	1.60	0.67
1:A:378:ASN:HD22	1:A:380:VAL:CG2	2.10	0.64
1:A:214:GLU:HG3	1:A:219:ILE:O	1.97	0.63
1:A:442:VAL:HG13	1:A:528:MET:CE	2.31	0.61
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.82	0.61
1:A:341:VAL:HG13	1:A:355:VAL:CG2	2.33	0.58
1:A:378:ASN:ND2	1:A:380:VAL:HG22	2.18	0.56
1:A:214:GLU:OE2	1:A:221:LEU:N	2.27	0.54
1:A:442:VAL:HG13	1:A:528:MET:HE1	1.90	0.54
1:A:247:ARG:HG2	1:A:247:ARG:NH1	2.14	0.53
1:A:484:ILE:HB	1:A:511:ILE:HG12	1.93	0.50
1:A:5:ALA:HB3	1:A:180:VAL:HG22	1.93	0.50
1:A:442:VAL:HG13	1:A:528:MET:HE3	1.94	0.49
1:A:524:HIS:HE1	5:A:2078:HOH:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASN:HA	1:A:379:PRO:HD3	1.91	0.46
1:A:62:GLN:O	1:A:66:LEU:HD23	2.15	0.46
1:A:102:ASN:ND2	1:A:104:PRO:HD2	2.31	0.46
1:A:22:VAL:HG11	1:A:95:ALA:HB2	1.97	0.46
1:A:364:PRO:HG2	1:A:510:TRP:NE1	2.31	0.45
1:A:421:LYS:HB3	1:A:424:GLU:HB3	2.00	0.44
1:A:72:ARG:HG3	1:A:72:ARG:NH1	2.25	0.43
1:A:112:LEU:O	1:A:117:PHE:HB2	2.19	0.42
1:A:156:VAL:HB	1:A:158:MET:HE3	2.01	0.42
1:A:193:ALA:O	1:A:198:MET:HB2	2.19	0.42
1:A:33:PRO:CG	1:A:80:VAL:HG21	2.45	0.42
1:A:476:ALA:HB2	4:A:1553:XM0:H3	2.02	0.42
1:A:72:ARG:HG2	1:A:73:LYS:N	2.35	0.41
1:A:442:VAL:HG21	1:A:447:ILE:HD11	2.03	0.41
1:A:477:CYS:HA	1:A:480:LEU:HD22	2.03	0.40
1:A:82:LEU:H	1:A:82:LEU:HD22	1.87	0.40
1:A:306:GLU:CD	1:A:306:GLU:H	2.29	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	547/549 (100%)	532 (97%)	13 (2%)	2 (0%)	30	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	LYS
1	A	268	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	474/474 (100%)	425 (90%)	49 (10%)	7 7

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	20	PHE
1	A	23	LEU
1	A	36	LEU
1	A	38	ASN
1	A	42	GLN
1	A	43	LYS
1	A	47	GLU
1	A	68	GLU
1	A	72	ARG
1	A	76	GLU
1	A	79	LYS
1	A	82	LEU
1	A	85	ASN
1	A	89	LYS
1	A	122	LEU
1	A	145[A]	MET
1	A	145[B]	MET
1	A	176	SER
1	A	191	LYS
1	A	211	LYS
1	A	216	VAL
1	A	222	LEU
1	A	247	ARG
1	A	253	VAL
1	A	283	GLN
1	A	341	VAL
1	A	350	GLU
1	A	359	ASN
1	A	369	MET

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Mol	Chain	Res	Type
1	A	375	ILE
1	A	376	LYS
1	A	378	ASN
1	A	399	GLN
1	A	401	LEU
1	A	417	LEU
1	A	422	VAL
1	A	423	CYS
1	A	424	GLU
1	A	428	LEU
1	A	431	ASN
1	A	432	SER
1	A	441	MET
1	A	442	VAL
1	A	448	GLN
1	A	456	LYS
1	A	480	LEU
1	A	521	ASP
1	A	530	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	85	ASN
1	A	102	ASN
1	A	146	HIS
1	A	233	ASN
1	A	378	ASN
1	A	420	HIS
1	A	452	GLN
1	A	505	GLN
1	A	524	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
3	DMS	A	1551	-	3,3,3	0.95	0	3,3,3	0.57	0
2	SO4	A	1548	-	4,4,4	0.33	0	6,6,6	0.18	0
2	SO4	A	1549	-	4,4,4	0.41	0	6,6,6	0.19	0
3	DMS	A	1550	-	3,3,3	0.94	0	3,3,3	0.74	0
4	XM0	A	1553	-	11,11,11	3.91	6 (54%)	12,15,15	1.74	2 (16%)
3	DMS	A	1552	-	3,3,3	0.41	0	3,3,3	0.58	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
4	XM0	A	1553	-	-	-	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1553	XM0	C6-C5	6.85	1.50	1.39
4	A	1553	XM0	C1-C6	5.68	1.48	1.38
4	A	1553	XM0	C3-C4	5.62	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1553	XM0	C2-C3	5.34	1.48	1.38
4	A	1553	XM0	C2-C1	3.50	1.45	1.38
4	A	1553	XM0	C5-C4	3.36	1.45	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1553	XM0	C7-C5-C4	-3.02	108.47	110.50
4	A	1553	XM0	C5-C7-C8	2.80	106.40	103.41

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
4	A	1553	XM0	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	547/549 (99%)	0.31	30 (5%)	30 31	25, 54, 91, 125	2 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	417	LEU	3.6
1	A	422	VAL	3.4
1	A	376	LYS	3.3
1	A	82	LEU	3.1
1	A	432	SER	3.1
1	A	71	CYS	2.9
1	A	423	CYS	2.9
1	A	429	PHE	2.8
1	A	23	LEU	2.7
1	A	80	VAL	2.6
1	A	195	ASP	2.5
1	A	223	ASN	2.3
1	A	83	PRO	2.3
1	A	416	VAL	2.3
1	A	377	ALA	2.3
1	A	79	LYS	2.3
1	A	86	PHE	2.3
1	A	372	LEU	2.2
1	A	22	VAL	2.2
1	A	38	ASN	2.2
1	A	2	THR	2.2
1	A	371	PRO	2.1
1	A	421	LYS	2.1
1	A	203	VAL	2.1
1	A	20	PHE	2.1
1	A	529	ASP	2.1
1	A	77	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	419	MET	2.0
1	A	19	VAL	2.0
1	A	194	ARG	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 oligosaccharides 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(Å ²)	Q<0.9
2	SO4	A	1549	5/5	0.76	0.09	128,133,134,134	0
3	DMS	A	1551	4/4	0.76	0.18	101,102,103,103	0
4	XM0	A	1553	10/10	0.76	0.18	81,83,85,86	0
3	DMS	A	1552	4/4	0.77	0.42	118,120,121,133	0
3	DMS	A	1550	4/4	0.82	0.17	87,89,92,94	0
2	SO4	A	1548	5/5	0.87	0.14	110,115,115,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.