



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:37 AM UTC

PDB ID : 4ZSM / pdb_00004zsm
Title : BACE crystal structure with bicyclic aminothiazine fragment
Authors : Timm, D.E.
Deposited on : 2015-05-13
Resolution : 1.96 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

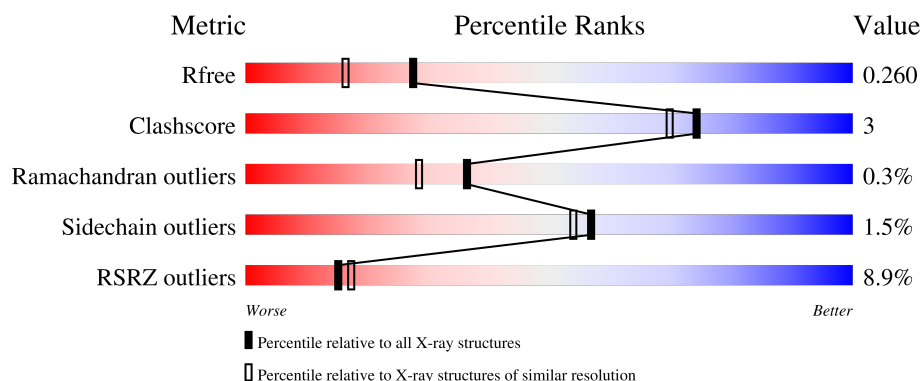
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 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	442	6% 80% 8% 12%
1	B	442	9% 79% 8% 12%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6633 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.

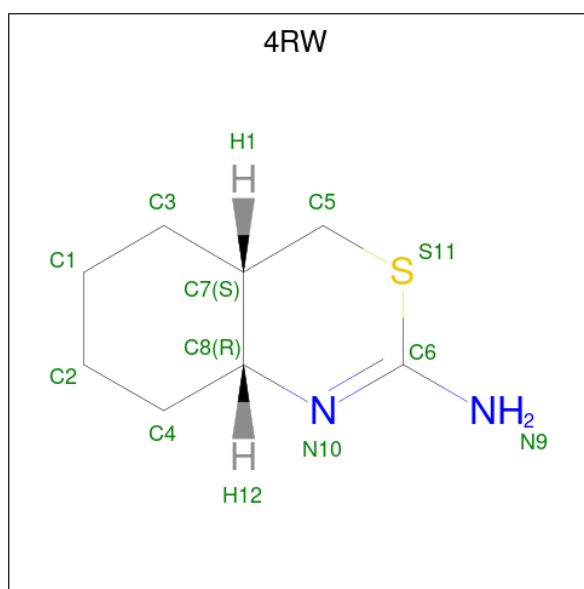
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	2	0
			3064	1962	510	578	14			
1	B	387	Total	C	N	O	S	0	1	0
			3050	1953	508	575	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-48	MET	-	initiating methionine	UNP P56817
B	-48	MET	-	initiating methionine	UNP P56817

- Molecule 2 is (4aS,8aR)-4a,5,6,7,8,8a-hexahydro-4H-3,1-benzothiazin-2-amine (CCD ID: 4RW) (formula: C₈H₁₄N₂S).



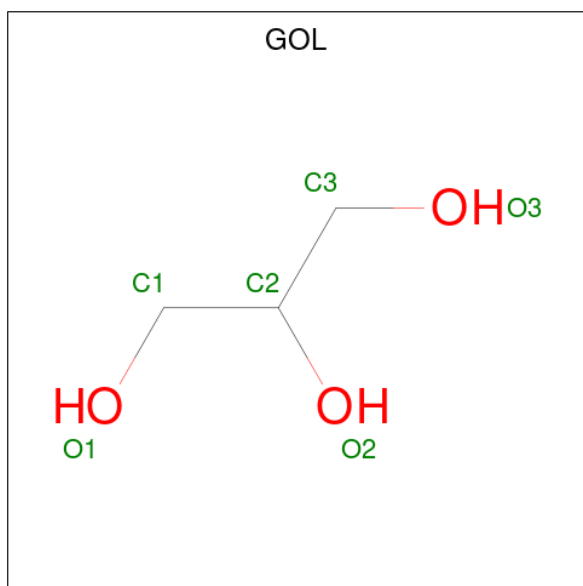
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			11	8	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	S	0	0
			11	8	2	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

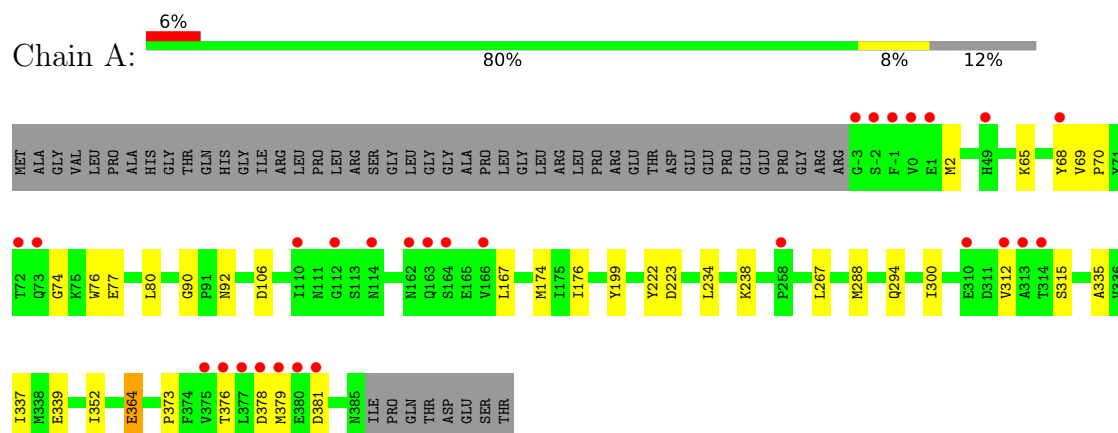
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	275	Total	O	0	0
			275	275		
4	B	215	Total	O	0	1
			216	216		

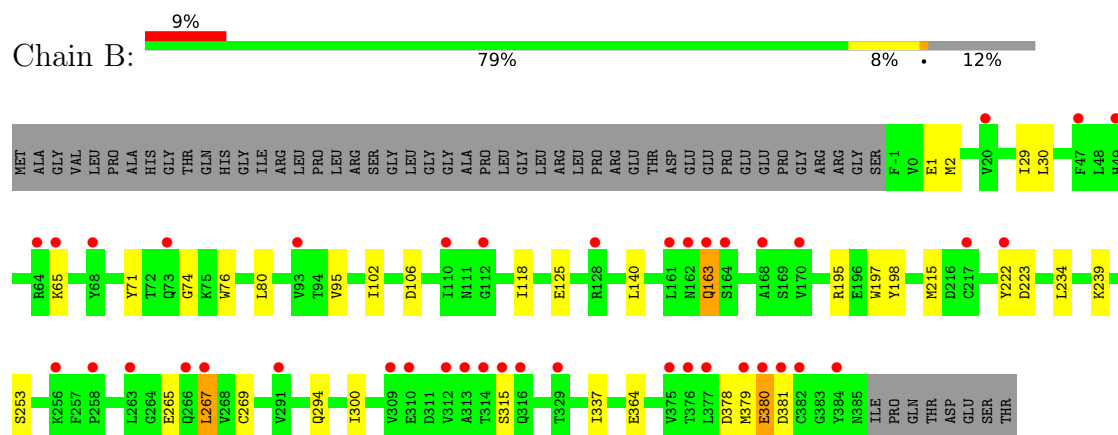
3 Residue-property plots [i](#)

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: Beta-secretase 1



• Molecule 1: Beta-secretase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.79Å 86.52Å 112.31Å 90.00° 97.62° 90.00°	Depositor
Resolution (Å)	26.50 – 1.96 26.50 – 1.96	Depositor EDS
% Data completeness (in resolution range)	96.7 (26.50-1.96) 96.7 (26.50-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.227 , 0.258 0.229 , 0.260	Depositor DCC
R_{free} test set	3633 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6633	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4RW, GOL

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	0.70	0/3148	0.86	0/4280
1	B	0.69	0/3131	0.87	3/4257 (0.1%)
All	All	0.70	0/6279	0.87	3/8537 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	GLN	N-CA-C	5.79	117.59	111.28
1	B	253	SER	N-CA-C	5.62	119.76	113.01
1	B	29	ILE	N-CA-C	5.45	115.71	107.75

There are no chirality outliers.

There are no planarity outliers.

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	3064	0	2984	19	0
1	B	3050	0	2967	19	0
2	A	11	0	14	0	0
2	B	11	0	14	1	0
3	A	6	0	8	0	0
4	A	275	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	216	0	0	1	0
All	All	6633	0	5987	38	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 (38) 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:B:300:ILE:HD13	1:B:337:ILE:HD12	1.71	0.72
1:B:125:GLU:OE2	1:B:195:ARG:NH2	2.25	0.69
1:A:300:ILE:HD13	1:A:337:ILE:HD12	1.75	0.68
1:B:378:ASP:O	1:B:381:ASP:HB2	1.97	0.64
1:A:174:MET:HE3	1:A:176:ILE:HD11	1.82	0.61
1:B:65:LYS:HE3	1:B:80:LEU:HD12	1.82	0.60
1:A:234:LEU:HB2	1:A:337:ILE:HD11	1.83	0.59
1:B:1:GLU:HG2	1:B:2:MET:HG3	1.85	0.58
1:A:68:TYR:HD1	1:A:77:GLU:HG2	1.70	0.57
1:A:288:MET:HE2	1:A:379:MET:HB3	1.87	0.56
1:B:265:GLU:HG2	4:B:713:HOH:O	2.06	0.55
1:B:380:GLU:H	1:B:380:GLU:CD	2.14	0.54
1:A:364:GLU:O	1:A:364:GLU:HG3	2.08	0.52
1:A:70:PRO:HD2	4:A:615:HOH:O	2.10	0.52
1:A:238:LYS:HE3	4:A:538:HOH:O	2.10	0.51
1:B:300:ILE:HD13	1:B:337:ILE:CD1	2.39	0.49
1:A:74:GLY:HA2	1:A:106:ASP:O	2.13	0.48
1:A:335:ALA:O	1:A:339:GLU:HG3	2.13	0.48
1:A:222:TYR:HA	1:A:223:ASP:HA	1.74	0.47
1:B:197:TRP:CG	1:B:198:TYR:H	2.33	0.46
1:B:30:LEU:HB3	1:B:118:ILE:HG22	1.98	0.46
1:B:234:LEU:HB2	1:B:337:ILE:HD11	1.98	0.46
1:B:222:TYR:HA	1:B:223:ASP:HA	1.69	0.45
1:B:215:MET:HE1	1:B:239:LYS:HB3	1.99	0.45
1:B:267:LEU:HD13	1:B:269:CYS:SG	2.57	0.45
1:A:199:TYR:HB3	1:A:352:ILE:HD11	1.97	0.44
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.99	0.43
1:A:300:ILE:HD13	1:A:337:ILE:CD1	2.46	0.43
1:B:74:GLY:HA2	1:B:106:ASP:O	2.19	0.43
1:A:65:LYS:HE3	1:A:80:LEU:HD12	2.01	0.42
1:B:294:GLN:O	1:B:379:MET:HE1	2.19	0.42
1:A:68:TYR:HD1	1:A:77:GLU:CG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:HB3	1:A:381:ASP:OD2	2.20	0.42
1:B:76:TRP:CE3	1:B:102:ILE:HG12	2.55	0.42
1:B:71:TYR:CZ	2:B:401:4RW:H7	2.56	0.41
1:A:294:GLN:HG2	1:A:373:PRO:HB2	2.03	0.41
1:A:69:VAL:HG21	1:A:76:TRP:CZ2	2.56	0.41
1:B:95:VAL:HG11	1:B:140:LEU:HA	2.02	0.41

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	389/442 (88%)	377 (97%)	11 (3%)	1 (0%)	36	28
1	B	386/442 (87%)	378 (98%)	7 (2%)	1 (0%)	36	28
All	All	775/884 (88%)	755 (97%)	18 (2%)	2 (0%)	36	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	SER
1	B	315	SER

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	333/373 (89%)	327 (98%)	6 (2%)	51	47
1	B	331/373 (89%)	327 (99%)	4 (1%)	63	61
All	All	664/746 (89%)	654 (98%)	10 (2%)	57	54

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	167	LEU
1	A	267	LEU
1	A	312	VAL
1	A	364	GLU
1	A	376	THR
1	B	163	GLN
1	B	267	LEU
1	B	364	GLU
1	B	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	A	294	GLN
1	A	385	ASN
1	B	89	HIS
1	B	114	ASN
1	B	163	GLN
1	B	233	ASN
1	B	266	GLN
1	B	385	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 oligosaccharides in this entry.

5.6 Ligand geometry

3 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	4RW	B	401	-	11,12,12	0.97	1 (9%)	9,16,16	1.80	3 (33%)
2	4RW	A	401	-	11,12,12	0.91	0	9,16,16	1.78	3 (33%)
3	GOL	A	402	-	5,5,5	1.00	0	5,5,5	0.53	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	4RW	B	401	-	-	-	0/2/2/2
2	4RW	A	401	-	-	-	0/2/2/2
3	GOL	A	402	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	4RW	C5-C7	-2.36	1.51	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	4RW	C8-N10-C6	2.90	120.21	115.61
2	B	401	4RW	S11-C6-N10	-2.86	125.73	129.93
2	B	401	4RW	C8-N10-C6	2.86	120.14	115.61
2	A	401	4RW	S11-C6-N10	-2.72	125.93	129.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	4RW	C4-C8-N10	-2.52	105.46	110.47
2	B	401	4RW	C4-C8-N10	-2.33	105.83	110.47

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	B	401	4RW	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	389/442 (88%)	0.65	28 (7%) 21 25	19, 28, 50, 72	2 (0%)
1	B	387/442 (87%)	0.80	41 (10%) 11 13	17, 31, 53, 72	1 (0%)
All	All	776/884 (87%)	0.73	69 (8%) 15 17	17, 30, 52, 72	3 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	VAL	6.5
1	B	314	THR	5.3
1	A	377	LEU	5.3
1	A	313	ALA	5.2
1	B	110	ILE	5.1
1	A	314	THR	4.9
1	A	312	VAL	4.8
1	A	110	ILE	4.3
1	A	163	GLN	4.2
1	A	-3	GLY	4.1
1	B	313	ALA	4.0
1	B	380	GLU	3.9
1	B	128	ARG	3.7
1	B	170	VAL	3.7
1	A	73	GLN	3.6
1	B	49	HIS	3.6
1	A	-2	SER	3.6
1	A	112	GLY	3.5
1	B	379	MET	3.4
1	A	0	VAL	3.3
1	A	379	MET	3.2
1	A	380	GLU	3.2
1	A	49	HIS	3.1
1	A	381	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	375	VAL	3.0
1	A	164	SER	3.0
1	A	166	VAL	2.9
1	B	384	TYR	2.9
1	B	217	CYS	2.8
1	B	258	PRO	2.8
1	B	68	TYR	2.7
1	B	315	SER	2.7
1	B	267	LEU	2.7
1	A	162	ASN	2.7
1	A	378	ASP	2.6
1	B	381	ASP	2.6
1	B	64	ARG	2.6
1	A	-1	PHE	2.6
1	A	376	THR	2.6
1	B	73	GLN	2.6
1	B	163	GLN	2.6
1	B	376	THR	2.5
1	B	263	LEU	2.5
1	B	377	LEU	2.5
1	B	93	VAL	2.5
1	A	1	GLU	2.5
1	B	162	ASN	2.4
1	B	310	GLU	2.4
1	B	164	SER	2.4
1	B	161	LEU	2.4
1	B	256	LYS	2.4
1	B	168	ALA	2.3
1	B	20	VAL	2.3
1	A	258	PRO	2.3
1	B	112	GLY	2.3
1	B	375	VAL	2.3
1	B	222	TYR	2.3
1	A	114	ASN	2.2
1	B	316	GLN	2.2
1	A	72	THR	2.2
1	B	382	CYS	2.2
1	B	329	THR	2.2
1	A	310	GLU	2.1
1	B	266	GLN	2.0
1	B	65	LYS	2.0
1	B	47	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	68	TYR	2.0
1	B	291	VAL	2.0
1	B	309	VAL	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
3	GOL	A	402	6/6	0.77	0.19	33,38,42,45	0
2	4RW	B	401	11/11	0.91	0.11	38,38,40,42	0
2	4RW	A	401	11/11	0.91	0.12	34,35,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.