



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:03 PM UTC

PDB ID : 2QCC / pdb_00002qcc
Title : Crystal structure of the orotidine-5'-monophosphate decarboxylase domain of human UMP synthase, apo form
Authors : Wittmann, J.; Rudolph, M.
Deposited on : 2007-06-19
Resolution : 1.85 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

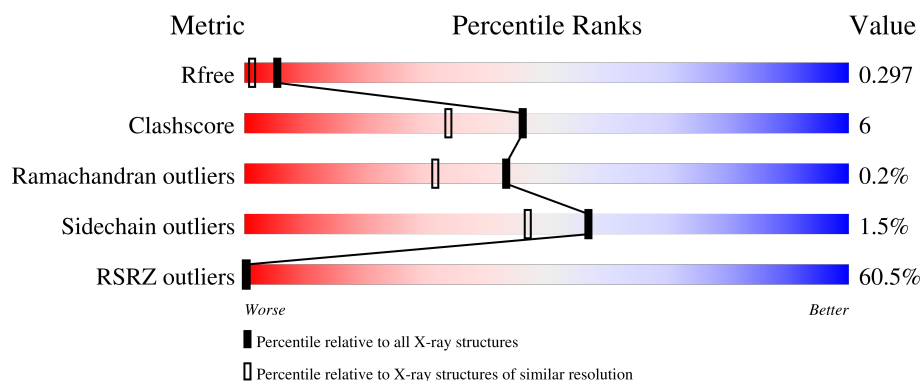
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	260	51% 83%12%5%
1	B	260	65% 85%11%.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4211 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.

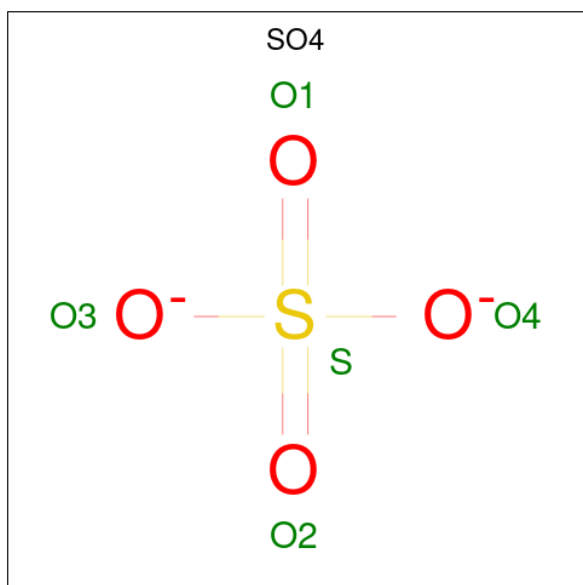
- Molecule 1 is a protein called Orotidine 5'- phosphate decarboxylase (OMPdecase).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	5	1
			1925	1228	331	354	12			
1	B	251	Total	C	N	O	S	0	9	2
			1959	1249	339	358	13			

There are 6 discrepancies between the modelled and reference sequences:

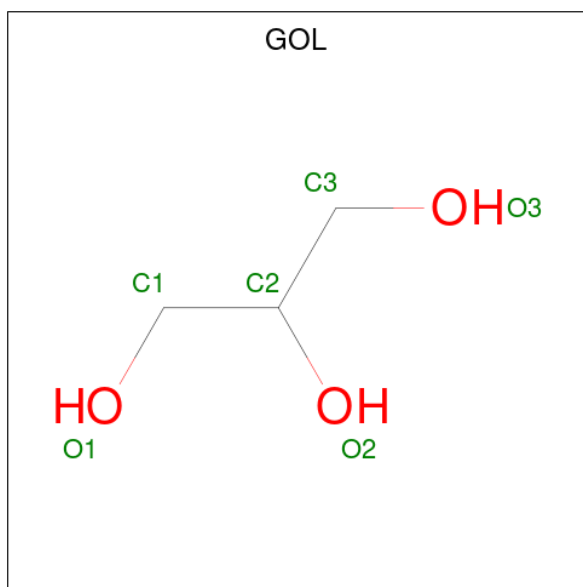
Chain	Residue	Modelled	Actual	Comment	Reference
A	221	GLY	-	expression tag	UNP P11172
A	222	ALA	-	expression tag	UNP P11172
A	223	MET	-	expression tag	UNP P11172
B	221	GLY	-	expression tag	UNP P11172
B	222	ALA	-	expression tag	UNP P11172
B	223	MET	-	expression tag	UNP P11172

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



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

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



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

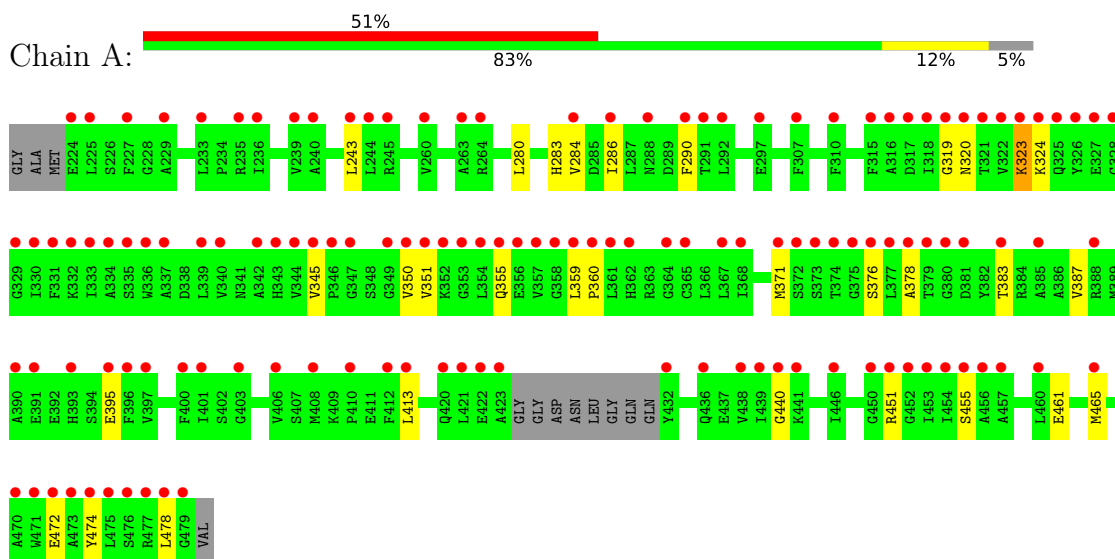
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	167	Total O 167 167	0	0
4	B	138	Total O 138 138	0	0

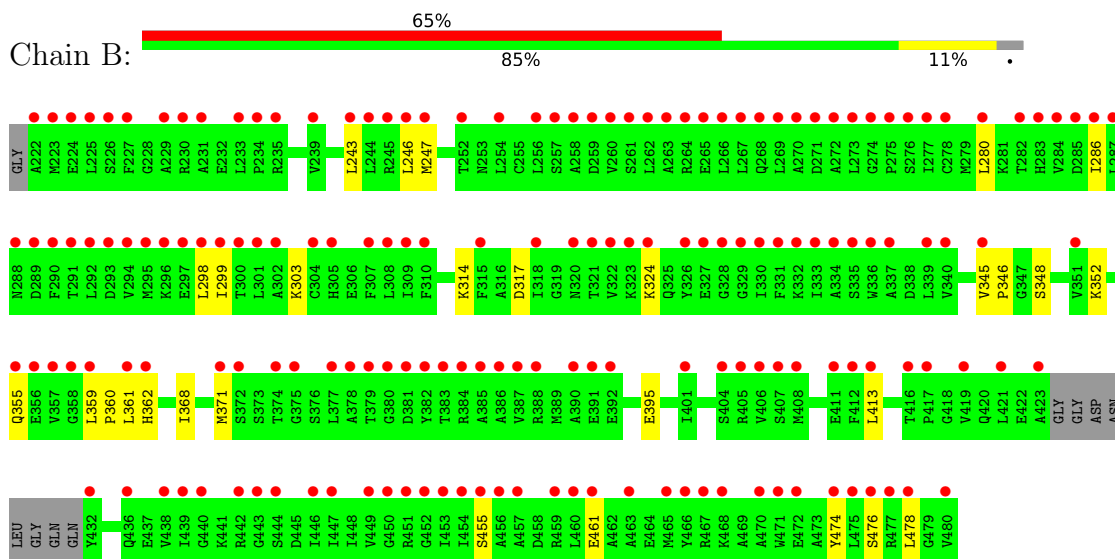
3 Residue-property plots

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: Orotidine 5'-phosphate decarboxylase (OMPdecase)



- Molecule 1: Orotidine 5'-phosphate decarboxylase (OMPdecase)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.02Å 75.91Å 119.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 1.85 46.96 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.96-1.85) 96.0 (46.96-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.258 (Not available) , 0.297	Depositor DCC
R_{free} test set	2352 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4211	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4597e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, 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	0.76	0/1971	0.83	0/2658
1	B	0.73	0/2017	0.83	0/2719
All	All	0.75	0/3988	0.83	0/5377

There are no bond length outliers.

There are no bond angle outliers.

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	1925	0	1983	29	0
1	B	1959	0	2030	23	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	167	0	0	5	0
4	B	138	0	0	4	0
All	All	4211	0	4029	46	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 (46) 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:371[A]:MET:HE2	4:B:576:HOH:O	1.58	1.03
1:A:324:LYS:HB3	1:B:286[A]:ILE:HG23	1.62	0.82
1:A:345:VAL:HG22	1:B:371:MET:HE1	1.68	0.75
1:A:371[A]:MET:HE1	4:B:507:HOH:O	1.91	0.68
1:B:474:TYR:CE1	1:B:478:LEU:HD11	2.36	0.60
1:B:474:TYR:O	1:B:478:LEU:HD13	2.02	0.60
1:A:286[A]:ILE:HG21	1:B:324:LYS:HD2	1.85	0.59
1:A:355:GLN:NE2	1:A:395:GLU:OE2	2.34	0.59
1:B:280:LEU:HD22	1:B:298:LEU:HD11	1.85	0.58
1:A:320:ASN:ND2	1:A:324:LYS:CE	2.68	0.57
1:A:324:LYS:CB	1:B:286[A]:ILE:HG23	2.35	0.57
1:B:395:GLU:H	1:B:395:GLU:CD	2.13	0.56
1:A:371[B]:MET:HB2	1:A:376:SER:OG	2.08	0.54
1:A:286[A]:ILE:HG23	1:B:324:LYS:HB3	1.89	0.54
1:B:455:SER:HB2	4:B:535:HOH:O	2.10	0.51
1:B:348:SER:OG	1:B:352:LYS:HE2	2.11	0.51
1:B:359:LEU:HB2	1:B:360:PRO:HD3	1.92	0.50
1:A:320:ASN:ND2	1:A:324:LYS:NZ	2.60	0.50
1:B:246:LEU:HD12	1:B:247:MET:N	2.27	0.50
1:B:345:VAL:HG12	1:B:346:PRO:HD3	1.94	0.50
1:A:472:GLU:HG2	4:A:615:HOH:O	2.13	0.49
1:B:243:LEU:HD23	1:B:413:LEU:HD13	1.95	0.49
1:A:359:LEU:HB2	1:A:360:PRO:HD3	1.95	0.48
1:A:320:ASN:HD22	1:A:324:LYS:NZ	2.11	0.48
1:A:350:VAL:HG13	1:A:351:VAL:N	2.29	0.47
1:A:345:VAL:HG22	1:B:371:MET:CE	2.40	0.47
1:A:284[A]:VAL:CG2	1:A:290:PHE:CD1	2.99	0.46
1:A:474:TYR:CE1	1:A:478:LEU:HD11	2.51	0.46
1:B:246:LEU:HD12	1:B:246:LEU:C	2.41	0.46
1:B:345:VAL:N	1:B:346:PRO:CD	2.79	0.46
1:A:319:GLY:O	1:A:323:LYS:HG3	2.17	0.45
1:A:371[A]:MET:CE	4:B:576:HOH:O	2.39	0.45
1:B:314:LYS:HG2	1:B:368:ILE:HD11	1.98	0.45
1:A:455:SER:HB2	4:A:602:HOH:O	2.16	0.45
1:A:320:ASN:ND2	1:A:324:LYS:HE2	2.32	0.44
1:B:299:ILE:O	1:B:303:LYS:HG3	2.18	0.42
1:A:461:GLU:O	1:A:465:MET:HG3	2.18	0.42
1:A:440:GLY:HA3	4:A:583:HOH:O	2.20	0.42
1:A:243:LEU:HD23	1:A:413:LEU:HD13	2.01	0.41
1:B:243:LEU:HD23	1:B:413:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:THR:O	1:A:387:VAL:HG23	2.21	0.41
1:A:451:ARG:NH2	4:A:540:HOH:O	2.54	0.41
1:B:361:LEU:C	1:B:362:HIS:CD2	2.99	0.41
1:A:283:HIS:HD2	4:A:485:HOH:O	2.03	0.40
1:B:345:VAL:CG1	1:B:346:PRO:HD3	2.52	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	249/260 (96%)	240 (96%)	8 (3%)	1 (0%)	30	17
1	B	256/260 (98%)	251 (98%)	5 (2%)	0	100	100
All	All	505/520 (97%)	491 (97%)	13 (3%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	ALA

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	208/210 (99%)	206 (99%)	2 (1%)	68 60
1	B	213/210 (101%)	209 (98%)	4 (2%)	50 38
All	All	421/420 (100%)	415 (99%)	6 (1%)	57 49

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	LEU
1	A	323	LYS
1	B	317	ASP
1	B	355	GLN
1	B	461	GLU
1	B	476	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	HIS
1	A	320	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	SO4	A	481	-	4,4,4	0.24	0	6,6,6	0.24	0
2	SO4	B	481	-	4,4,4	0.17	0	6,6,6	0.35	0
3	GOL	A	482	-	5,5,5	0.39	0	5,5,5	0.18	0
3	GOL	B	482	-	5,5,5	0.42	0	5,5,5	0.85	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	GOL	A	482	-	-	2/4/4/4	-
3	GOL	B	482	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	482	GOL	C1-C2-C3-O3
3	A	482	GOL	O2-C2-C3-O3

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 ⓘ

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	248/260 (95%)	2.21	132 (53%) 0 0	26, 43, 50, 54	5 (2%)
1	B	251/260 (96%)	2.59	170 (67%) 0 0	25, 43, 51, 67	9 (3%)
All	All	499/520 (95%)	2.40	302 (60%) 0 0	25, 43, 50, 67	14 (2%)

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	MET	6.7
1	A	423	ALA	6.7
1	B	222	ALA	6.3
1	B	290	PHE	5.7
1	B	286[A]	ILE	5.5
1	B	291	THR	5.3
1	A	438	VAL	5.2
1	B	423	ALA	5.2
1	B	294	VAL	4.9
1	B	284	VAL	4.9
1	B	328	GLY	4.8
1	B	460	LEU	4.8
1	B	331	PHE	4.7
1	B	476	SER	4.7
1	B	227	PHE	4.6
1	B	453	ILE	4.6
1	B	408	MET	4.6
1	B	361	LEU	4.5
1	B	260	VAL	4.5
1	B	263	ALA	4.4
1	A	321	THR	4.4
1	A	354	LEU	4.3
1	B	292	LEU	4.3
1	B	264	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	478	LEU	4.2
1	B	273	LEU	4.2
1	B	480	VAL	4.2
1	A	361	LEU	4.2
1	A	359	LEU	4.2
1	A	357	VAL	4.1
1	B	266	LEU	4.1
1	B	320[A]	ASN	4.1
1	A	297	GLU	4.1
1	B	451[A]	ARG	4.0
1	A	479	GLY	4.0
1	A	451	ARG	4.0
1	A	362	HIS	4.0
1	A	322	VAL	4.0
1	B	302	ALA	4.0
1	B	470	ALA	4.0
1	B	440	GLY	4.0
1	B	287	LEU	4.0
1	A	319	GLY	3.9
1	B	262	LEU	3.9
1	B	454	ILE	3.9
1	B	388	ARG	3.9
1	B	333	ILE	3.9
1	A	358	GLY	3.9
1	B	362	HIS	3.9
1	A	377	LEU	3.8
1	B	258	ALA	3.8
1	B	461	GLU	3.8
1	B	298	LEU	3.7
1	B	324	LYS	3.7
1	B	226	SER	3.7
1	B	330	ILE	3.7
1	B	336	TRP	3.7
1	B	301	LEU	3.7
1	A	318	ILE	3.7
1	A	345	VAL	3.7
1	B	288	ASN	3.7
1	A	323	LYS	3.7
1	A	360	PRO	3.6
1	B	378	ALA	3.6
1	A	350	VAL	3.6
1	B	225	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	478	LEU	3.5
1	A	432	TYR	3.5
1	B	269	LEU	3.5
1	B	455	SER	3.5
1	B	474	TYR	3.5
1	B	234	PRO	3.5
1	A	324	LYS	3.5
1	A	376	SER	3.4
1	A	396	PHE	3.4
1	B	233	LEU	3.4
1	A	455	SER	3.4
1	B	261[A]	SER	3.4
1	B	267	LEU	3.4
1	B	438	VAL	3.4
1	B	256	LEU	3.4
1	B	265[A]	GLU	3.3
1	A	320	ASN	3.3
1	A	351	VAL	3.3
1	B	276	SER	3.3
1	A	356	GLU	3.3
1	B	268	GLN	3.3
1	A	239	VAL	3.3
1	A	406	VAL	3.3
1	A	470	ALA	3.3
1	B	297	GLU	3.2
1	B	465[A]	MET	3.2
1	A	233	LEU	3.2
1	A	471	TRP	3.2
1	B	272	ALA	3.2
1	B	277	ILE	3.2
1	B	299	ILE	3.2
1	B	307	PHE	3.2
1	A	374	THR	3.1
1	B	387	VAL	3.1
1	A	355	GLN	3.1
1	B	439	ILE	3.1
1	B	359	LEU	3.1
1	A	290	PHE	3.1
1	B	282	THR	3.1
1	B	379	THR	3.1
1	B	375	GLY	3.1
1	A	326	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	375	GLY	3.1
1	A	441	LYS	3.0
1	A	284[A]	VAL	3.0
1	B	372	SER	3.0
1	A	353	GLY	3.0
1	A	390	ALA	3.0
1	B	300	THR	3.0
1	B	329	GLY	3.0
1	A	224	GLU	3.0
1	B	280	LEU	3.0
1	B	432	TYR	3.0
1	A	412	PHE	3.0
1	A	334	ALA	3.0
1	A	339	LEU	2.9
1	B	405	ARG	2.9
1	A	403	GLY	2.9
1	A	331	PHE	2.9
1	B	457	ALA	2.9
1	A	236	ILE	2.9
1	B	335	SER	2.9
1	B	477	ARG	2.9
1	A	349	GLY	2.9
1	A	472	GLU	2.9
1	B	380	GLY	2.9
1	B	270	ALA	2.9
1	B	296	LYS	2.9
1	A	286[A]	ILE	2.9
1	B	246	LEU	2.9
1	B	475	LEU	2.9
1	A	395	GLU	2.9
1	A	340	VAL	2.9
1	B	239	VAL	2.9
1	A	264	ARG	2.9
1	B	332	LYS	2.9
1	A	476	SER	2.9
1	B	224	GLU	2.9
1	B	295	MET	2.9
1	B	308	LEU	2.9
1	A	316	ALA	2.8
1	A	473	ALA	2.8
1	A	421	LEU	2.8
1	B	254	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	466	TYR	2.8
1	B	411	GLU	2.8
1	A	240	ALA	2.8
1	A	347	GLY	2.8
1	A	330	ILE	2.8
1	B	245	ARG	2.8
1	B	283	HIS	2.8
1	A	410	PRO	2.8
1	B	285	ASP	2.8
1	A	342	ALA	2.8
1	A	457	ALA	2.8
1	B	337	ALA	2.8
1	A	245	ARG	2.8
1	A	393	HIS	2.8
1	A	460	LEU	2.8
1	B	293	ASP	2.8
1	B	345	VAL	2.8
1	A	364	GLY	2.7
1	B	443	GLY	2.7
1	A	454	ILE	2.7
1	B	278	CYS	2.7
1	B	304	CYS	2.7
1	B	412	PHE	2.7
1	B	406	VAL	2.7
1	B	229	ALA	2.7
1	B	463	ALA	2.7
1	B	416	THR	2.7
1	A	388	ARG	2.7
1	A	367	LEU	2.7
1	A	439	ILE	2.7
1	A	260	VAL	2.7
1	A	465	MET	2.6
1	A	379	THR	2.6
1	A	400	PHE	2.6
1	B	356	GLU	2.6
1	B	275	PRO	2.6
1	A	244	LEU	2.6
1	A	328	GLY	2.6
1	B	274	GLY	2.6
1	B	471	TRP	2.6
1	A	378	ALA	2.6
1	A	397	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	436[A]	GLN	2.6
1	A	422	GLU	2.6
1	A	456	ALA	2.6
1	B	259	ASP	2.5
1	A	336	TRP	2.5
1	A	352	LYS	2.5
1	B	446	ILE	2.5
1	A	383	THR	2.5
1	B	392	GLU	2.5
1	A	315	PHE	2.5
1	B	315	PHE	2.5
1	A	401	ILE	2.5
1	B	231	ALA	2.5
1	B	334	ALA	2.5
1	B	371	MET	2.5
1	B	450	GLY	2.5
1	A	329	GLY	2.4
1	B	235	ARG	2.4
1	B	377	LEU	2.4
1	B	257	SER	2.4
1	A	333	ILE	2.4
1	A	332	LYS	2.4
1	B	289	ASP	2.4
1	B	419	VAL	2.4
1	A	477	ARG	2.4
1	B	459	ARG	2.4
1	B	472	GLU	2.4
1	A	371[A]	MET	2.4
1	B	404	SER	2.4
1	B	358	GLY	2.4
1	A	225	LEU	2.4
1	B	374	THR	2.4
1	B	309	ILE	2.4
1	B	447	ILE	2.4
1	A	263	ALA	2.4
1	A	343	HIS	2.4
1	B	305	HIS	2.4
1	B	444	SER	2.4
1	A	408	MET	2.3
1	B	323	LYS	2.3
1	A	373	SER	2.3
1	A	327	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	292	LEU	2.3
1	B	243	LEU	2.3
1	B	339	LEU	2.3
1	B	252	THR	2.3
1	B	321	THR	2.3
1	B	326	TYR	2.3
1	A	229	ALA	2.3
1	A	337	ALA	2.3
1	B	386	ALA	2.3
1	A	453	ILE	2.3
1	B	417	PRO	2.3
1	A	440	GLY	2.3
1	A	452	GLY	2.3
1	B	351	VAL	2.3
1	A	475	LEU	2.3
1	A	446	ILE	2.3
1	A	413	LEU	2.3
1	B	421	LEU	2.3
1	A	310	PHE	2.2
1	A	380	GLY	2.2
1	A	391	GLU	2.2
1	B	407	SER	2.2
1	A	235	ARG	2.2
1	B	383	THR	2.2
1	A	317	ASP	2.2
1	A	436	GLN	2.2
1	A	474	TYR	2.2
1	B	382	TYR	2.2
1	B	391	GLU	2.2
1	A	420	GLN	2.2
1	A	381	ASP	2.2
1	B	456	ALA	2.2
1	A	227	PHE	2.2
1	B	401	ILE	2.2
1	B	327	GLU	2.2
1	B	322	VAL	2.2
1	B	390	ALA	2.2
1	B	468	LYS	2.2
1	A	368	ILE	2.1
1	B	318	ILE	2.1
1	B	449	VAL	2.1
1	A	335	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	450	GLY	2.1
1	A	365	CYS	2.1
1	B	230	ARG	2.1
1	B	413	LEU	2.1
1	A	385	ALA	2.1
1	B	357	VAL	2.1
1	B	384	ARG	2.1
1	B	452	GLY	2.1
1	A	288	ASN	2.1
1	B	244	LEU	2.1
1	A	325	GLN	2.1
1	B	385	ALA	2.1
1	B	310	PHE	2.1
1	B	381	ASP	2.1
1	B	467	ARG	2.1
1	A	291	THR	2.1
1	A	344	VAL	2.1
1	A	307	PHE	2.0
1	A	372	SER	2.0
1	B	355	GLN	2.0
1	B	340	VAL	2.0
1	A	243	LEU	2.0
1	B	271	ASP	2.0
1	B	442	ARG	2.0
1	B	247	MET	2.0
1	A	346	PRO	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($\text{\AA}^2$)	Q<0.9
3	GOL	A	482	6/6	0.78	0.23	47,51,52,52	0
3	GOL	B	482	6/6	0.79	0.21	47,53,53,54	0
2	SO4	A	481	5/5	0.93	0.15	57,58,58,59	0
2	SO4	B	481	5/5	0.93	0.15	54,55,57,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.