



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:13 PM UTC

PDB ID : 3R31 / pdb_00003r31
Title : Crystal structure of betaine aldehyde dehydrogenase from *Agrobacterium tumefaciens*
Authors : Agarwal, R.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on : 2011-03-15
Resolution : 2.15 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

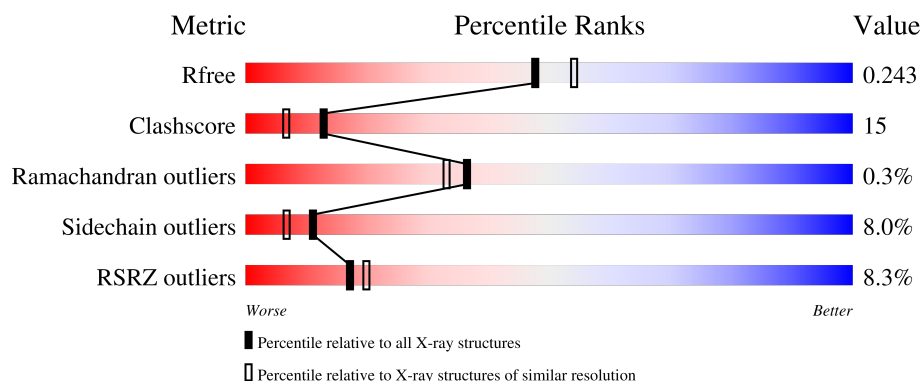
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

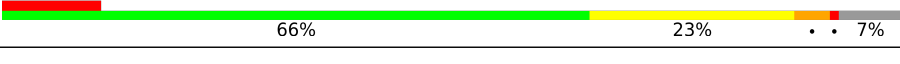
The reported resolution of this entry is 2.15 Å.

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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	517	
1	B	517	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7360 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 Betaine aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3575	2264	610	685	16			
1	B	482	Total	C	N	O	S	0	0	0
			3558	2251	610	681	16			

There are 48 discrepancies between the modelled and reference sequences:

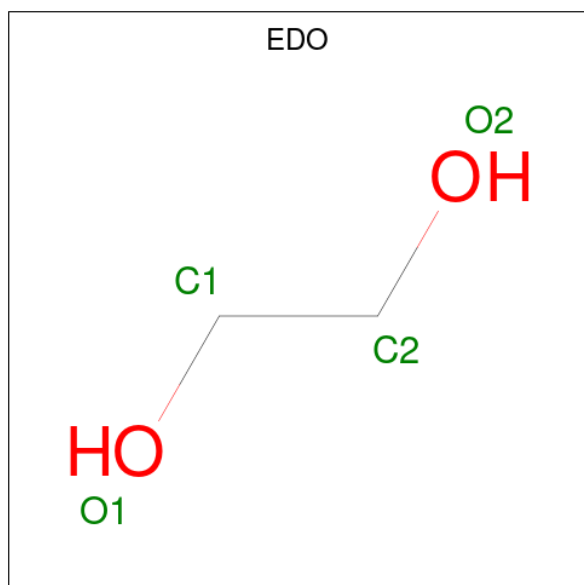
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q8UH56
A	2	VAL	-	expression tag	UNP Q8UH56
A	496	ALA	-	expression tag	UNP Q8UH56
A	497	GLU	-	expression tag	UNP Q8UH56
A	498	ASN	-	expression tag	UNP Q8UH56
A	499	LEU	-	expression tag	UNP Q8UH56
A	500	TYR	-	expression tag	UNP Q8UH56
A	501	PHE	-	expression tag	UNP Q8UH56
A	502	GLN	-	expression tag	UNP Q8UH56
A	503	SER	-	expression tag	UNP Q8UH56
A	504	HIS	-	expression tag	UNP Q8UH56
A	505	HIS	-	expression tag	UNP Q8UH56
A	506	HIS	-	expression tag	UNP Q8UH56
A	507	HIS	-	expression tag	UNP Q8UH56
A	508	HIS	-	expression tag	UNP Q8UH56
A	509	HIS	-	expression tag	UNP Q8UH56
A	510	TRP	-	expression tag	UNP Q8UH56
A	511	SER	-	expression tag	UNP Q8UH56
A	512	HIS	-	expression tag	UNP Q8UH56
A	513	PRO	-	expression tag	UNP Q8UH56
A	514	GLN	-	expression tag	UNP Q8UH56
A	515	PHE	-	expression tag	UNP Q8UH56
A	516	GLU	-	expression tag	UNP Q8UH56
A	517	LYS	-	expression tag	UNP Q8UH56
B	1	MET	-	expression tag	UNP Q8UH56

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	VAL	-	expression tag	UNP Q8UH56
B	496	ALA	-	expression tag	UNP Q8UH56
B	497	GLU	-	expression tag	UNP Q8UH56
B	498	ASN	-	expression tag	UNP Q8UH56
B	499	LEU	-	expression tag	UNP Q8UH56
B	500	TYR	-	expression tag	UNP Q8UH56
B	501	PHE	-	expression tag	UNP Q8UH56
B	502	GLN	-	expression tag	UNP Q8UH56
B	503	SER	-	expression tag	UNP Q8UH56
B	504	HIS	-	expression tag	UNP Q8UH56
B	505	HIS	-	expression tag	UNP Q8UH56
B	506	HIS	-	expression tag	UNP Q8UH56
B	507	HIS	-	expression tag	UNP Q8UH56
B	508	HIS	-	expression tag	UNP Q8UH56
B	509	HIS	-	expression tag	UNP Q8UH56
B	510	TRP	-	expression tag	UNP Q8UH56
B	511	SER	-	expression tag	UNP Q8UH56
B	512	HIS	-	expression tag	UNP Q8UH56
B	513	PRO	-	expression tag	UNP Q8UH56
B	514	GLN	-	expression tag	UNP Q8UH56
B	515	PHE	-	expression tag	UNP Q8UH56
B	516	GLU	-	expression tag	UNP Q8UH56
B	517	LYS	-	expression tag	UNP Q8UH56

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

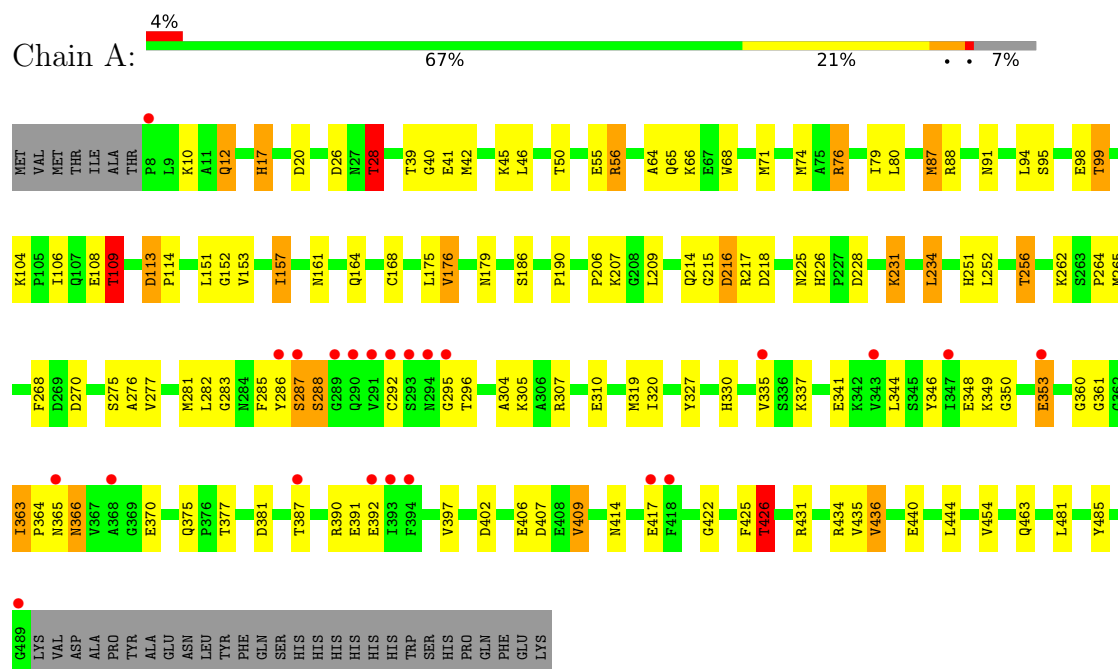
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total 117	O 117	0	0
3	B	102	Total 102	O 102	0	0

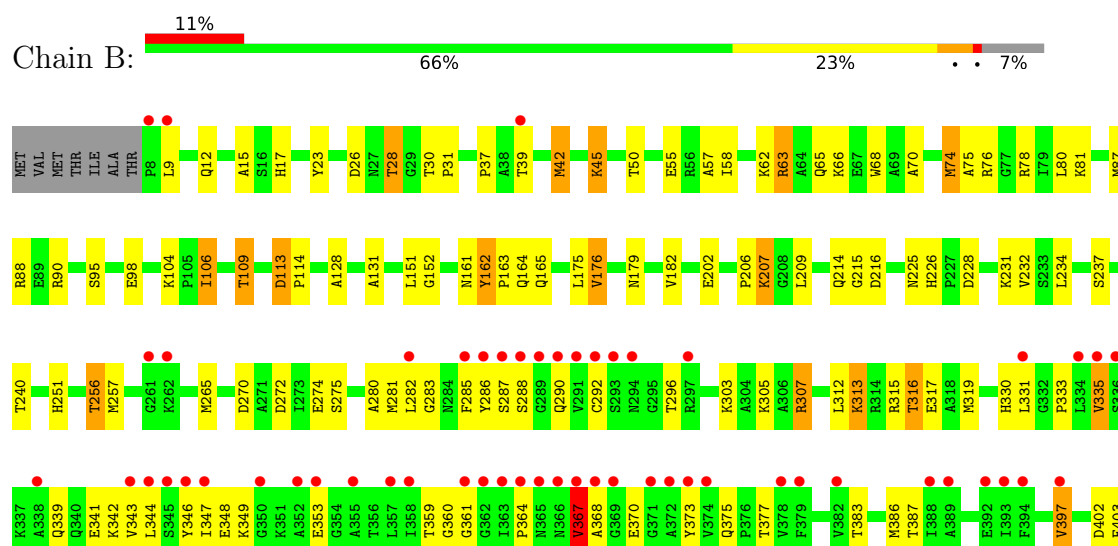
3 Residue-property plots [i](#)

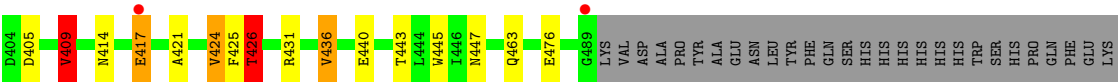
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Betaine aldehyde dehydrogenase



• Molecule 1: Betaine aldehyde dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.88Å 98.88Å 174.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.02 – 2.15 43.02 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.02-2.15) 99.9 (43.02-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.194 , 0.245 0.197 , 0.243	Depositor DCC
R_{free} test set	2767 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7360	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: 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	1.38	15/3648 (0.4%)	1.25	24/4954 (0.5%)
1	B	1.31	15/3630 (0.4%)	1.22	14/4931 (0.3%)
All	All	1.35	30/7278 (0.4%)	1.23	38/9885 (0.4%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	VAL	C-O	-7.30	1.15	1.24
1	B	75	ALA	C-O	-7.29	1.15	1.24
1	A	176	VAL	C-O	-7.24	1.15	1.24
1	A	87	MET	SD-CE	-6.99	1.62	1.79
1	A	74	MET	C-O	-6.32	1.16	1.24
1	B	74	MET	SD-CE	6.05	1.94	1.79
1	A	335	VAL	CA-CB	6.00	1.61	1.54
1	A	66	LYS	C-O	-5.94	1.17	1.24
1	B	88	ARG	C-O	-5.92	1.17	1.24
1	B	62	LYS	C-O	-5.86	1.17	1.24
1	B	57	ALA	C-O	-5.80	1.17	1.24
1	B	367	VAL	CA-CB	-5.80	1.46	1.54
1	A	175	LEU	C-O	-5.71	1.17	1.24
1	B	63	ARG	C-O	-5.70	1.17	1.24
1	B	368	ALA	CA-CB	-5.65	1.44	1.53
1	B	70	ALA	C-O	-5.63	1.17	1.24
1	A	79	ILE	C-O	-5.58	1.17	1.24
1	A	91	ASN	C-O	-5.54	1.17	1.24
1	A	88	ARG	C-O	-5.51	1.17	1.24
1	B	87	MET	C-O	-5.51	1.17	1.24
1	B	131	ALA	C-O	-5.40	1.17	1.24
1	B	476	GLU	C-O	-5.38	1.17	1.24
1	A	71	MET	CB-CG	5.17	1.68	1.52
1	A	76	ARG	C-O	-5.14	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	ALA	C-O	-5.14	1.19	1.24
1	A	217	ARG	C-O	-5.11	1.17	1.24
1	A	17	HIS	C-O	-5.08	1.17	1.23
1	A	281	MET	C-O	-5.07	1.18	1.24
1	A	153	VAL	CA-CB	5.07	1.60	1.54
1	B	175	LEU	C-O	-5.01	1.18	1.24

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	VAL	N-CA-C	-9.08	102.36	112.80
1	A	409	VAL	CB-CA-C	-8.60	100.52	112.14
1	B	426	THR	CB-CA-C	-7.93	95.65	110.16
1	A	12	GLN	CA-C-N	-7.77	112.83	120.52
1	A	12	GLN	C-N-CA	-7.77	112.83	120.52
1	A	286	TYR	N-CA-C	-7.59	102.98	111.71
1	B	237	SER	CA-C-N	7.47	124.94	120.24
1	B	237	SER	C-N-CA	7.47	124.94	120.24
1	A	215	GLY	N-CA-C	7.30	122.43	111.18
1	A	28	THR	N-CA-CB	-6.43	101.07	110.53
1	B	215	GLY	N-CA-C	6.41	120.51	110.96
1	B	409	VAL	CB-CA-C	-6.39	103.40	112.22
1	A	65	GLN	N-CA-C	6.32	118.17	111.28
1	A	426	THR	CB-CA-C	-6.24	96.66	109.94
1	B	436	VAL	CB-CA-C	6.21	120.52	112.14
1	B	335	VAL	N-CA-C	6.01	116.48	110.23
1	A	409	VAL	N-CA-C	5.96	116.70	110.62
1	B	128	ALA	CA-C-N	-5.89	113.59	120.12
1	B	128	ALA	C-N-CA	-5.89	113.59	120.12
1	A	363	ILE	N-CA-C	-5.75	103.68	108.63
1	A	109	THR	CB-CA-C	5.69	120.24	110.79
1	A	10	LYS	N-CA-C	5.66	118.18	111.33
1	A	28	THR	N-CA-C	-5.63	106.58	113.50
1	B	162	TYR	CB-CA-C	5.53	115.13	111.20
1	A	277	VAL	N-CA-C	5.53	115.72	110.42
1	A	186	SER	CA-C-N	5.46	127.60	120.28
1	A	186	SER	C-N-CA	5.46	127.60	120.28
1	A	327	TYR	N-CA-C	5.46	119.04	112.38
1	A	287	SER	N-CA-C	5.44	118.20	110.10
1	A	481	LEU	CA-C-N	-5.43	115.23	122.72
1	A	481	LEU	C-N-CA	-5.43	115.23	122.72
1	A	109	THR	N-CA-CB	-5.32	102.29	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	THR	CA-C-N	5.31	125.99	119.99
1	B	240	THR	C-N-CA	5.31	125.99	119.99
1	A	217	ARG	N-CA-C	-5.27	105.65	111.71
1	B	424	VAL	CB-CA-C	-5.20	102.73	110.33
1	A	390	ARG	N-CA-C	5.11	116.66	111.14
1	A	64	ALA	N-CA-C	5.10	117.74	111.82

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	3575	0	3543	98	0
1	B	3558	0	3519	118	0
2	A	4	0	6	1	0
2	B	4	0	6	0	0
3	A	117	0	0	3	0
3	B	102	0	0	5	0
All	All	7360	0	7074	215	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 15.

All (215) 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:42:MET:CE	1:A:45:LYS:HG2	1.66	1.24
1:A:426:THR:HG21	1:A:431:ARG:HD2	1.16	1.08
1:A:42:MET:HE3	1:A:45:LYS:HG2	1.39	1.03
1:B:364:PRO:HG2	1:B:367:VAL:HG21	1.40	1.03
1:B:307:ARG:HG3	1:B:307:ARG:HH11	1.25	1.00
1:A:42:MET:CE	1:A:45:LYS:CG	2.39	0.99
1:B:364:PRO:CG	1:B:367:VAL:HG21	1.93	0.98
1:B:316:THR:HG21	1:B:359:THR:HG21	1.47	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLN:HE22	1:B:45:LYS:H	1.12	0.92
1:B:113:ASP:HB3	1:B:114:PRO:HD3	1.52	0.91
1:A:12:GLN:HE22	1:A:45:LYS:H	1.19	0.90
1:B:226:HIS:HD2	1:B:228:ASP:H	1.17	0.90
1:B:364:PRO:HB2	1:B:367:VAL:CG2	2.02	0.90
1:A:426:THR:CG2	1:A:431:ARG:HD2	2.03	0.88
1:A:226:HIS:HD2	1:A:228:ASP:H	1.24	0.85
1:A:349:LYS:O	1:A:353:GLU:CG	2.23	0.85
1:A:42:MET:HE1	1:A:45:LYS:HG2	1.59	0.84
1:B:285:PHE:CD2	1:B:319:MET:HE1	2.12	0.83
1:A:349:LYS:O	1:A:353:GLU:HG2	1.79	0.82
1:B:42:MET:HE1	1:B:45:LYS:HG3	1.59	0.82
1:B:364:PRO:CB	1:B:367:VAL:HG21	2.10	0.81
1:B:344:LEU:O	1:B:348:GLU:HG2	1.80	0.81
1:B:417:GLU:CG	1:B:463:GLN:HG3	2.11	0.80
1:A:113:ASP:HB3	1:A:114:PRO:HD3	1.63	0.80
1:B:316:THR:CG2	1:B:317:GLU:N	2.45	0.80
1:A:231:LYS:NZ	1:A:256:THR:HB	1.97	0.79
1:B:426:THR:HG21	1:B:431:ARG:HD2	1.66	0.78
1:B:417:GLU:HG2	1:B:463:GLN:HG3	1.66	0.78
1:A:320:ILE:H	1:A:330:HIS:HD2	1.31	0.77
1:B:364:PRO:HB2	1:B:367:VAL:HG21	1.64	0.77
1:B:66:LYS:HE2	1:B:66:LYS:HA	1.67	0.77
1:B:281:MET:HE3	1:B:319:MET:HE2	1.67	0.76
1:B:316:THR:HG22	1:B:317:GLU:N	2.00	0.76
1:A:307:ARG:HG3	1:A:307:ARG:HH11	1.51	0.76
1:A:231:LYS:HZ1	1:A:256:THR:HB	1.50	0.76
1:A:151:LEU:H	1:A:179:ASN:HD21	1.31	0.75
1:B:364:PRO:HB2	1:B:367:VAL:HG22	1.68	0.74
1:B:364:PRO:HG2	1:B:367:VAL:CG2	2.18	0.74
1:B:414:ASN:HD21	1:B:440:GLU:H	1.36	0.74
1:B:113:ASP:HB3	1:B:114:PRO:CD	2.20	0.72
1:A:349:LYS:O	1:A:353:GLU:HG3	1.90	0.71
1:B:58:ILE:HD13	1:B:182:VAL:HG21	1.74	0.70
1:A:361:GLY:H	1:A:377:THR:CG2	2.03	0.70
1:A:414:ASN:HD21	1:A:440:GLU:H	1.39	0.69
1:B:417:GLU:CD	1:B:463:GLN:HG3	2.17	0.69
1:B:426:THR:CG2	1:B:431:ARG:HD2	2.23	0.69
1:B:349:LYS:O	1:B:353:GLU:HG3	1.92	0.68
1:B:353:GLU:OE2	1:B:387:THR:HB	1.93	0.68
1:B:361:GLY:H	1:B:377:THR:CG2	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LYS:HG2	1:A:295:GLY:O	1.95	0.67
1:A:265:MET:HE3	1:A:425:PHE:CE2	2.28	0.67
1:B:285:PHE:C	1:B:287:SER:H	2.03	0.67
1:B:361:GLY:H	1:B:377:THR:HG22	1.59	0.67
1:B:26:ASP:OD2	1:B:28:THR:HB	1.95	0.67
1:A:104:LYS:NZ	1:A:288:SER:HB3	2.12	0.65
1:B:274:GLU:O	1:B:315:ARG:NH2	2.28	0.65
1:A:375:GLN:O	1:A:377:THR:HG23	1.97	0.65
1:A:42:MET:HE2	1:A:45:LYS:CG	2.25	0.64
1:B:42:MET:CE	1:B:45:LYS:HG3	2.27	0.64
1:A:226:HIS:CD2	1:A:228:ASP:H	2.10	0.64
1:B:417:GLU:OE2	1:B:463:GLN:HB2	1.98	0.64
1:A:360:GLY:HA3	1:A:377:THR:HG22	1.81	0.63
1:A:406:GLU:OE2	1:A:434:ARG:HD2	1.99	0.62
1:B:256:THR:HG21	3:B:615:HOH:O	1.99	0.62
1:B:17:HIS:HD2	1:B:214:GLN:H	1.45	0.62
1:B:226:HIS:CD2	1:B:228:ASP:H	2.08	0.62
1:A:17:HIS:HD2	1:A:214:GLN:H	1.46	0.61
1:A:426:THR:HG21	1:A:431:ARG:CD	2.11	0.61
1:A:113:ASP:CB	1:A:114:PRO:HD3	2.31	0.61
1:B:364:PRO:CB	1:B:367:VAL:CG2	2.71	0.61
1:B:231:LYS:HZ3	1:B:256:THR:HB	1.65	0.60
1:A:95:SER:HB3	1:A:109:THR:HG23	1.82	0.60
1:A:113:ASP:HB3	1:A:114:PRO:CD	2.30	0.60
1:B:307:ARG:HH11	1:B:307:ARG:CG	2.09	0.60
1:B:316:THR:HG22	1:B:317:GLU:H	1.65	0.60
1:A:55:GLU:OE1	1:A:226:HIS:HE1	1.85	0.59
1:A:305:LYS:HD2	1:A:402:ASP:OD1	2.02	0.59
1:B:63:ARG:HD2	3:B:595:HOH:O	2.01	0.59
1:A:305:LYS:NZ	1:A:381:ASP:OD1	2.36	0.58
1:B:106:ILE:HG13	1:B:106:ILE:O	2.02	0.58
1:B:165:GLN:HE21	1:B:290:GLN:HE21	1.51	0.58
1:B:353:GLU:OE2	1:B:387:THR:CB	2.51	0.58
1:A:225:ASN:HD22	1:A:251:HIS:CD2	2.22	0.58
1:A:270:ASP:OD1	1:A:426:THR:HG22	2.04	0.58
1:B:151:LEU:H	1:B:179:ASN:HD21	1.52	0.58
1:B:68:TRP:CE2	1:B:76:ARG:HD2	2.39	0.57
1:B:307:ARG:HG3	1:B:307:ARG:NH1	2.05	0.57
1:A:414:ASN:ND2	1:A:440:GLU:H	2.01	0.57
1:B:206:PRO:HD2	1:B:209:LEU:HD12	1.87	0.57
1:A:417:GLU:HG2	1:A:463:GLN:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:SER:HB3	1:B:109:THR:HG23	1.87	0.57
1:B:207:LYS:HG2	3:B:574:HOH:O	2.05	0.56
1:A:26:ASP:OD2	1:A:28:THR:HB	2.05	0.56
1:A:361:GLY:H	1:A:377:THR:HG21	1.69	0.56
1:B:375:GLN:O	1:B:377:THR:HG23	2.06	0.56
1:B:65:GLN:NE2	1:B:66:LYS:HE3	2.20	0.55
1:A:108:GLU:OE2	1:A:288:SER:OG	2.24	0.55
1:B:65:GLN:HE22	1:B:66:LYS:HE3	1.71	0.55
1:B:360:GLY:HA3	1:B:377:THR:HG22	1.89	0.55
1:B:403:PHE:CG	1:B:409:VAL:HG13	2.41	0.55
1:B:17:HIS:CD2	1:B:214:GLN:H	2.24	0.55
1:A:17:HIS:CD2	1:A:214:GLN:H	2.24	0.54
2:A:3318:EDO:H21	3:A:569:HOH:O	2.07	0.53
1:B:9:LEU:HD12	1:B:9:LEU:H	1.72	0.53
1:B:417:GLU:HG2	1:B:463:GLN:CG	2.37	0.53
1:A:68:TRP:CE2	1:A:76:ARG:HD2	2.44	0.53
1:A:42:MET:HE1	1:A:45:LYS:CG	2.26	0.53
1:A:262:LYS:HG2	1:A:295:GLY:C	2.33	0.53
1:A:252:LEU:HD12	1:B:463:GLN:NE2	2.24	0.52
1:A:265:MET:HE1	1:A:276:ALA:O	2.09	0.52
1:A:152:GLY:H	1:A:179:ASN:HD22	1.57	0.52
1:B:55:GLU:OE1	1:B:226:HIS:HE1	1.92	0.52
1:B:78:ARG:NH1	3:B:609:HOH:O	2.32	0.51
1:A:320:ILE:H	1:A:330:HIS:CD2	2.21	0.51
1:A:361:GLY:H	1:A:377:THR:HG22	1.75	0.51
1:B:335:VAL:HG23	1:B:339:GLN:HG3	1.92	0.51
1:A:426:THR:CG2	1:A:431:ARG:HH11	2.23	0.51
1:B:285:PHE:C	1:B:287:SER:N	2.67	0.51
1:B:414:ASN:ND2	1:B:440:GLU:H	2.06	0.51
1:B:319:MET:HA	1:B:330:HIS:HD2	1.74	0.51
1:A:283:GLY:HA2	1:A:292:CYS:SG	2.51	0.51
1:A:151:LEU:N	1:A:179:ASN:HD21	2.05	0.51
1:A:39:THR:C	1:A:41:GLU:H	2.19	0.50
1:B:312:LEU:O	1:B:316:THR:HB	2.10	0.50
1:A:216:ASP:HB3	1:A:218:ASP:H	1.76	0.50
1:B:95:SER:HB3	1:B:109:THR:CG2	2.41	0.50
1:B:225:ASN:HD22	1:B:251:HIS:CD2	2.30	0.50
1:A:98:GLU:HG2	1:A:164:GLN:OE1	2.11	0.49
1:B:98:GLU:HG2	1:B:164:GLN:OE1	2.11	0.49
1:B:37:PRO:HB3	1:B:335:VAL:HA	1.93	0.49
1:A:94:LEU:HB3	1:A:164:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:PRO:O	1:A:365:ASN:OD1	2.30	0.49
1:A:42:MET:HE2	1:A:45:LYS:HG3	1.95	0.48
1:B:74:MET:O	1:B:74:MET:HG3	2.11	0.48
1:B:68:TRP:CH2	1:B:76:ARG:HG2	2.48	0.48
1:A:285:PHE:HB3	1:A:319:MET:HE1	1.95	0.48
1:B:421:ALA:HA	1:B:443:THR:O	2.14	0.48
1:A:346:TYR:CE1	1:A:397:VAL:HG21	2.48	0.48
1:B:15:ALA:HB3	1:B:23:TYR:HB3	1.95	0.48
1:A:417:GLU:OE2	1:A:463:GLN:HB2	2.14	0.48
1:A:307:ARG:HG3	1:A:307:ARG:NH1	2.26	0.47
1:A:406:GLU:OE1	1:A:434:ARG:NH1	2.47	0.47
1:A:206:PRO:HD2	1:A:209:LEU:HD12	1.96	0.47
1:B:98:GLU:OE1	1:B:163:PRO:HD2	2.14	0.47
1:B:152:GLY:H	1:B:179:ASN:HD22	1.62	0.47
1:B:63:ARG:CD	3:B:595:HOH:O	2.61	0.47
1:B:346:TYR:CE1	1:B:397:VAL:HG21	2.50	0.47
1:A:444:LEU:N	1:A:444:LEU:HD22	2.30	0.46
1:B:283:GLY:HA2	1:B:292:CYS:SG	2.55	0.46
1:B:313:LYS:O	1:B:316:THR:HG22	2.15	0.46
1:A:106:ILE:HD12	1:A:109:THR:CG2	2.45	0.46
1:A:353:GLU:OE2	1:A:387:THR:N	2.48	0.46
1:A:285:PHE:C	1:A:287:SER:N	2.72	0.46
1:B:417:GLU:CD	1:B:463:GLN:HB2	2.40	0.46
1:B:425:PHE:HA	1:B:447:ASN:OD1	2.16	0.46
1:A:113:ASP:CB	1:A:114:PRO:CD	2.93	0.46
1:A:350:GLY:HA2	1:A:353:GLU:HG3	1.98	0.46
1:B:39:THR:HA	1:B:370:GLU:HB2	1.98	0.45
1:B:65:GLN:HE22	1:B:66:LYS:CE	2.30	0.45
1:B:12:GLN:HE22	1:B:45:LYS:N	1.95	0.45
1:B:383:THR:H	1:B:386:MET:HG3	1.82	0.45
1:B:333:PRO:HD3	1:B:373:TYR:CE1	2.51	0.45
1:B:231:LYS:HG3	1:B:232:VAL:N	2.31	0.45
1:B:265:MET:HE1	1:B:280:ALA:HB2	1.99	0.45
1:B:316:THR:HA	1:B:319:MET:HE3	1.97	0.45
1:B:335:VAL:CG2	1:B:339:GLN:HG3	2.47	0.45
1:A:304:ALA:O	1:A:305:LYS:C	2.60	0.44
1:B:305:LYS:HD2	1:B:402:ASP:OD1	2.16	0.44
1:B:417:GLU:CD	1:B:463:GLN:CB	2.90	0.44
1:A:436:VAL:HG22	1:A:444:LEU:HB3	2.00	0.44
1:B:316:THR:HG23	1:B:317:GLU:N	2.30	0.44
1:B:162:TYR:N	1:B:163:PRO:HD3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:O	1:A:348:GLU:HG2	2.17	0.44
1:A:42:MET:HE1	1:A:45:LYS:CD	2.47	0.44
1:A:365:ASN:HA	1:A:366:ASN:HA	1.78	0.44
1:B:30:THR:HA	1:B:31:PRO:HD3	1.93	0.44
1:A:56:ARG:HD2	3:A:571:HOH:O	2.18	0.44
1:A:17:HIS:HE1	3:A:580:HOH:O	2.01	0.43
1:A:282:LEU:O	1:A:287:SER:CA	2.66	0.43
1:B:151:LEU:N	1:B:179:ASN:HD21	2.16	0.43
1:B:417:GLU:CD	1:B:463:GLN:CG	2.90	0.43
1:A:28:THR:HG22	1:A:50:THR:HG21	1.99	0.43
1:B:165:GLN:NE2	1:B:290:GLN:HE21	2.17	0.43
1:A:152:GLY:H	1:A:179:ASN:ND2	2.16	0.43
1:B:257:MET:HB3	1:B:257:MET:HE2	1.68	0.43
1:A:417:GLU:CG	1:A:463:GLN:HG3	2.49	0.43
1:B:113:ASP:CB	1:B:114:PRO:HD3	2.37	0.43
1:A:39:THR:C	1:A:41:GLU:N	2.77	0.43
1:A:485:TYR:HB3	1:B:445:TRP:CD1	2.53	0.43
1:B:234:LEU:HB3	1:B:257:MET:HE2	2.01	0.43
1:A:106:ILE:HD12	1:A:109:THR:HG22	2.01	0.42
1:B:270:ASP:OD2	1:B:426:THR:HG22	2.18	0.42
1:A:264:PRO:O	1:A:422:GLY:HA2	2.20	0.42
1:A:46:LEU:CD1	1:A:190:PRO:HG3	2.49	0.42
1:A:346:TYR:HE1	1:A:397:VAL:HG21	1.84	0.42
1:A:157:ILE:HB	1:A:234:LEU:HD12	2.01	0.42
1:A:431:ARG:O	1:A:435:VAL:HG23	2.19	0.42
1:B:342:LYS:HE2	1:B:342:LYS:HB3	1.83	0.42
1:B:272:ASP:OD1	1:B:272:ASP:C	2.63	0.41
1:B:316:THR:HG22	1:B:317:GLU:HG3	2.01	0.41
1:A:231:LYS:HZ1	1:A:256:THR:CG2	2.32	0.41
1:B:81:LYS:HB2	1:B:81:LYS:HE3	1.91	0.41
1:B:90:ARG:NH2	1:B:202:GLU:OE1	2.50	0.41
1:B:28:THR:HG22	1:B:50:THR:HG21	2.02	0.41
1:B:95:SER:O	1:B:109:THR:HG21	2.19	0.41
1:B:343:VAL:O	1:B:347:ILE:HG12	2.20	0.41
1:A:99:THR:OG1	1:A:109:THR:HG21	2.21	0.41
1:A:417:GLU:OE2	1:A:463:GLN:CB	2.69	0.41
1:B:216:ASP:OD1	1:B:216:ASP:C	2.63	0.41
1:A:337:LYS:O	1:A:341:GLU:HG2	2.21	0.41
1:B:104:LYS:HD3	1:B:104:LYS:HA	1.88	0.41
1:A:87:MET:HE1	1:A:168:CYS:SG	2.62	0.40
1:B:343:VAL:O	1:B:346:TYR:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:TYR:CD1	1:A:485:TYR:C	3.00	0.40
1:A:268:PHE:HB2	1:A:426:THR:HG23	2.03	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	480/517 (93%)	463 (96%)	15 (3%)	2 (0%)	30	26
1	B	480/517 (93%)	458 (95%)	21 (4%)	1 (0%)	43	42
All	All	960/1034 (93%)	921 (96%)	36 (4%)	3 (0%)	36	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	B	113	ASP
1	A	40	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	364/400 (91%)	335 (92%)	29 (8%)	11	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	360/400 (90%)	331 (92%)	29 (8%)	11	6
All	All	724/800 (90%)	666 (92%)	58 (8%)	11	7

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	28	THR
1	A	56	ARG
1	A	80	LEU
1	A	99	THR
1	A	109	THR
1	A	157	ILE
1	A	161	ASN
1	A	176	VAL
1	A	207	LYS
1	A	216	ASP
1	A	231	LYS
1	A	234	LEU
1	A	256	THR
1	A	275	SER
1	A	288	SER
1	A	296	THR
1	A	310	GLU
1	A	353	GLU
1	A	363	ILE
1	A	366	ASN
1	A	370	GLU
1	A	391	GLU
1	A	392	GLU
1	A	407	ASP
1	A	409	VAL
1	A	426	THR
1	A	436	VAL
1	A	454	VAL
1	B	28	THR
1	B	42	MET
1	B	45	LYS
1	B	80	LEU
1	B	106	ILE
1	B	109	THR
1	B	161	ASN

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Mol	Chain	Res	Type
1	B	176	VAL
1	B	207	LYS
1	B	256	THR
1	B	275	SER
1	B	282	LEU
1	B	286	TYR
1	B	288	SER
1	B	296	THR
1	B	303	LYS
1	B	307	ARG
1	B	313	LYS
1	B	316	THR
1	B	331	LEU
1	B	341	GLU
1	B	367	VAL
1	B	397	VAL
1	B	405	ASP
1	B	409	VAL
1	B	417	GLU
1	B	424	VAL
1	B	426	THR
1	B	436	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	17	HIS
1	A	65	GLN
1	A	161	ASN
1	A	164	GLN
1	A	165	GLN
1	A	179	ASN
1	A	188	ASN
1	A	225	ASN
1	A	226	HIS
1	A	290	GLN
1	A	330	HIS
1	A	366	ASN
1	A	414	ASN
1	A	450	ASN
1	A	477	HIS

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Mol	Chain	Res	Type
1	B	12	GLN
1	B	17	HIS
1	B	65	GLN
1	B	107	GLN
1	B	161	ASN
1	B	179	ASN
1	B	226	HIS
1	B	290	GLN
1	B	294	ASN
1	B	330	HIS
1	B	414	ASN
1	B	450	ASN
1	B	463	GLN
1	B	477	HIS

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](#)

2 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	EDO	A	3318	-	3,3,3	0.87	0	2,2,2	0.58	0
2	EDO	B	3319	-	3,3,3	1.28	0	2,2,2	0.26	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	EDO	A	3318	-	-	0/1/1/1	-
2	EDO	B	3319	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

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	A	3318	EDO	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	482/517 (93%)	0.07	23 (4%)	35 41	17, 30, 63, 76	0
1	B	482/517 (93%)	0.41	57 (11%)	9 11	17, 37, 75, 87	0
All	All	964/1034 (93%)	0.24	80 (8%)	17 20	17, 34, 71, 87	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	367	VAL	5.6
1	B	368	ALA	5.3
1	B	293	SER	4.9
1	A	8	PRO	4.6
1	B	335	VAL	4.6
1	B	394	PHE	4.5
1	A	353	GLU	4.4
1	B	291	VAL	4.4
1	A	368	ALA	4.3
1	A	286	TYR	4.1
1	B	289	GLY	3.8
1	A	289	GLY	3.7
1	B	8	PRO	3.6
1	B	344	LEU	3.6
1	A	293	SER	3.5
1	B	288	SER	3.5
1	B	392	GLU	3.5
1	B	343	VAL	3.4
1	B	346	TYR	3.4
1	B	352	ALA	3.4
1	A	394	PHE	3.4
1	B	361	GLY	3.2
1	B	292	CYS	3.2
1	B	287	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	295	GLY	3.2
1	B	358	ILE	3.2
1	A	292	CYS	3.2
1	B	372	ALA	3.1
1	B	366	ASN	3.1
1	B	261	GLY	3.1
1	B	355	ALA	3.1
1	B	290	GLN	3.1
1	B	369	GLY	3.0
1	B	388	ILE	3.0
1	B	371	GLY	2.9
1	B	297	ARG	2.9
1	A	387	THR	2.9
1	B	393	ILE	2.9
1	A	291	VAL	2.8
1	A	294	ASN	2.7
1	B	338	ALA	2.7
1	B	353	GLU	2.7
1	A	393	ILE	2.6
1	B	286	TYR	2.6
1	B	294	ASN	2.6
1	B	336	SER	2.6
1	A	392	GLU	2.6
1	A	489	GLY	2.6
1	B	389	ALA	2.5
1	B	347	ILE	2.5
1	B	365	ASN	2.5
1	B	397	VAL	2.4
1	B	345	SER	2.4
1	B	378	VAL	2.4
1	A	417	GLU	2.4
1	B	350	GLY	2.4
1	B	382	VAL	2.4
1	B	374	VAL	2.3
1	B	39	THR	2.3
1	A	290	GLN	2.3
1	A	365	ASN	2.3
1	A	347	ILE	2.3
1	B	334	LEU	2.3
1	B	373	TYR	2.3
1	B	9	LEU	2.3
1	B	363	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	364	PRO	2.2
1	B	489	GLY	2.2
1	B	331	LEU	2.1
1	A	287	SER	2.1
1	A	418	PHE	2.1
1	B	285	PHE	2.1
1	B	379	PHE	2.1
1	B	417	GLU	2.0
1	B	282	LEU	2.0
1	B	262	LYS	2.0
1	B	362	GLY	2.0
1	A	335	VAL	2.0
1	A	343	VAL	2.0
1	B	357	LEU	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
2	EDO	B	3319	4/4	0.75	0.19	37,42,43,44	0
2	EDO	A	3318	4/4	0.84	0.14	29,31,33,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.