



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:03 AM UTC

PDB ID : 1AFW / pdb_00001afw
Title : THE 1.8 ANGSTROM CRYSTAL STRUCTURE OF THE DIMERIC PEROXISOMAL THIOLASE OF SACCHAROMYCES CEREVISIAE
Authors : Mathieu, M.; Wierenga, R.K.
Deposited on : 1997-03-15
Resolution : 1.80 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

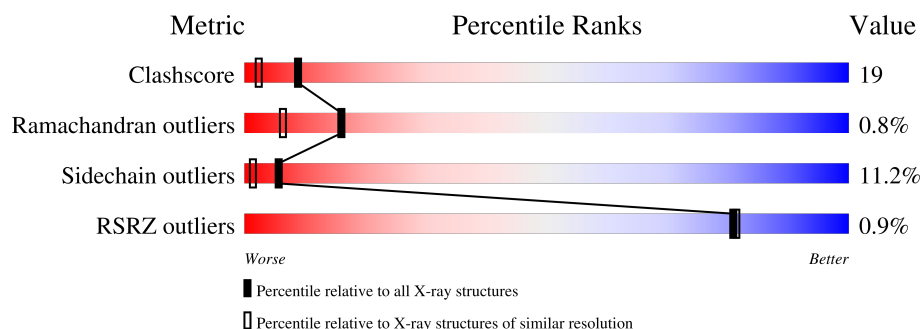
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	393	57% 34% 7% ..
1	B	393	56% 33% 9% .

2 Entry composition [i](#)

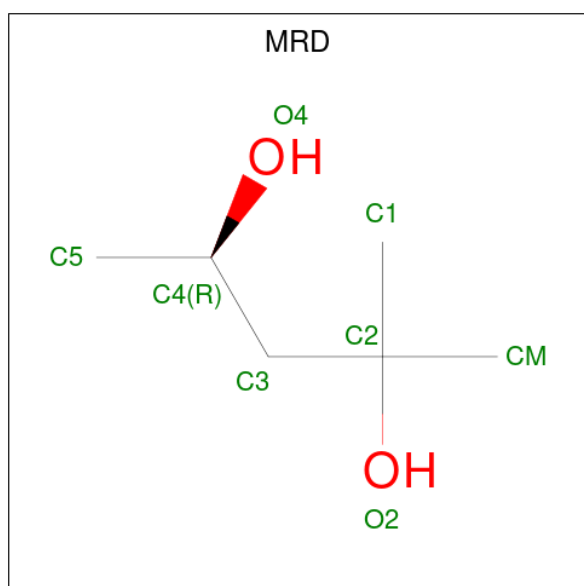
There are 3 unique types of molecules in this entry. The entry contains 6338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-KETOACETYL-COA THIOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			2923	1841	509	559	14			
1	B	393	Total	C	N	O	S	0	0	0
			2951	1857	516	564	14			

- Molecule 2 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		

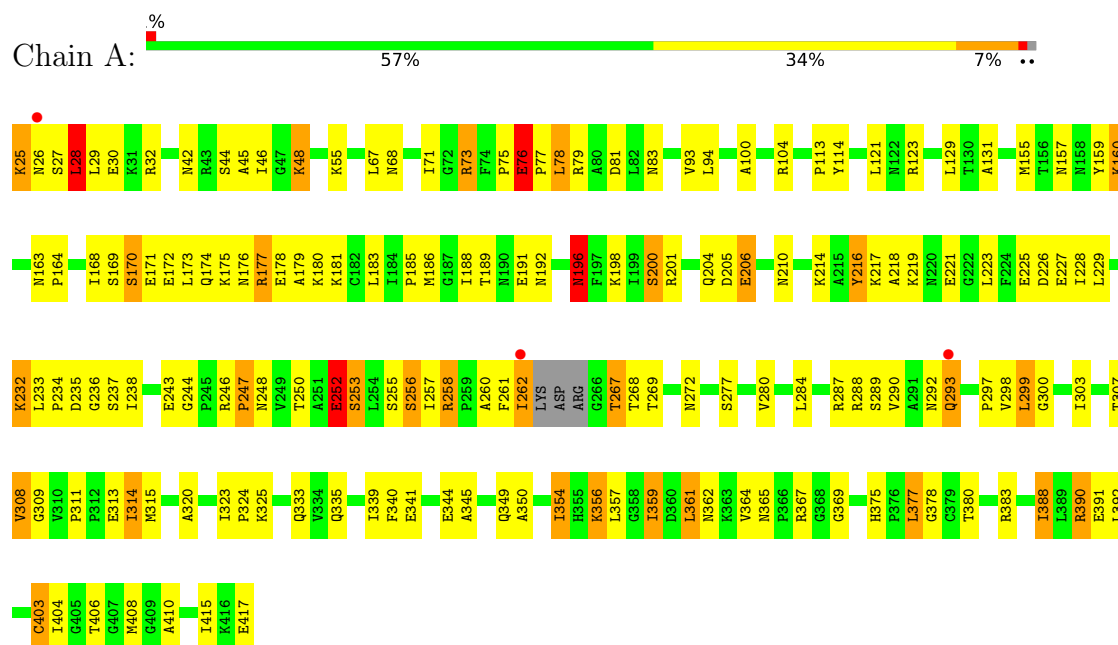
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	208	Total 208	O 208	0	0
3	B	240	Total 240	O 240	0	0

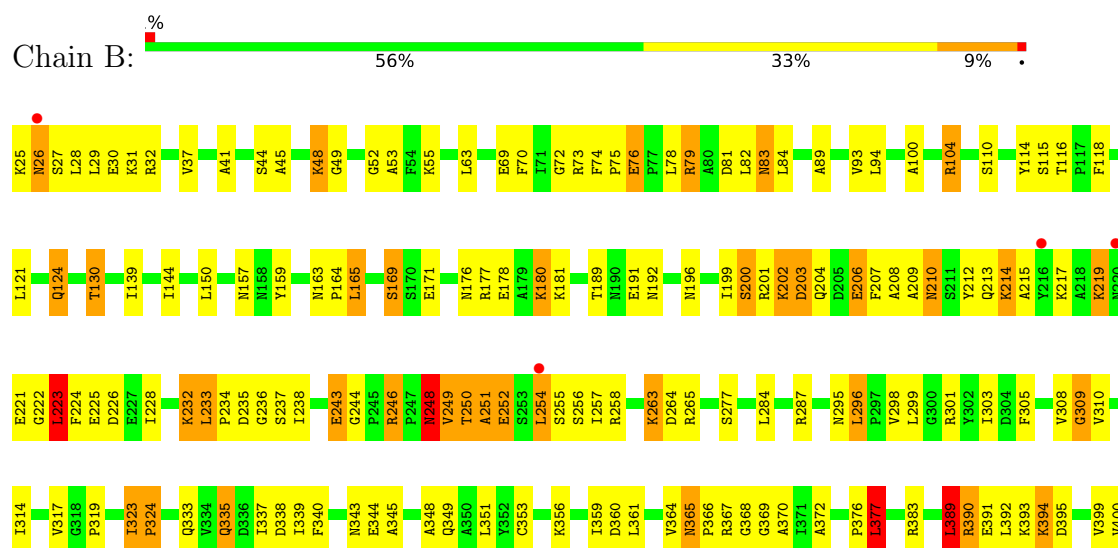
3 Residue-property plots

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: 3-KETOACETYL-COA THIOLASE



• Molecule 1: 3-KETOACETYL-COA THIOLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.17Å 92.65Å 116.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 10.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (10.00-1.80) 98.9 (10.00-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.34 (at 1.80Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.203 , 0.240 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 137.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6338	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: MRD

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	1.19	4/2966 (0.1%)	1.74	51/4013 (1.3%)
1	B	1.23	5/2995 (0.2%)	1.82	65/4052 (1.6%)
All	All	1.21	9/5961 (0.2%)	1.78	116/8065 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	THR	CA-CB	7.28	1.64	1.53
1	B	93	VAL	CA-CB	7.18	1.63	1.54
1	B	144	ILE	CA-CB	7.05	1.65	1.55
1	B	309	GLY	CA-C	5.93	1.58	1.52
1	A	131	ALA	CA-CB	5.93	1.62	1.53
1	A	359	ILE	CA-CB	5.53	1.61	1.54
1	B	41	ALA	CA-CB	-5.48	1.41	1.53
1	A	247	PRO	CA-C	5.32	1.58	1.53
1	B	310	VAL	C-O	5.32	1.28	1.24

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	PHE	N-CA-C	-9.79	98.91	114.09
1	B	214	LYS	N-CA-C	9.75	121.91	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	LEU	N-CA-C	9.71	125.33	113.38
1	A	196	ASN	N-CA-C	9.71	122.88	111.71
1	A	123	ARG	N-CA-C	-9.55	98.97	110.44
1	B	244	GLY	N-CA-C	9.24	131.19	112.34
1	A	248	ASN	N-CA-C	9.21	124.47	113.23
1	B	45	ALA	N-CA-C	-8.95	98.98	110.53
1	B	345	ALA	N-CA-C	-8.96	101.47	111.14
1	A	388	ILE	N-CA-C	8.82	120.67	110.62
1	A	44	SER	N-CA-C	-8.73	96.83	110.36
1	B	208	ALA	N-CA-C	8.67	120.73	111.28
1	A	45	ALA	N-CA-C	-8.47	99.11	110.55
1	B	55	LYS	N-CA-C	8.40	121.50	111.33
1	B	44	SER	N-CA-C	-8.16	97.71	110.36
1	B	228	ILE	N-CA-C	7.79	119.18	108.89
1	B	104	ARG	N-CA-C	-7.76	102.77	111.07
1	B	159	TYR	N-CA-C	-7.71	102.85	111.71
1	A	367	ARG	N-CA-C	-7.65	102.46	112.41
1	A	403	CYS	N-CA-C	-7.63	100.69	110.53
1	B	52	GLY	N-CA-C	7.62	125.10	112.30
1	B	263	LYS	N-CA-C	7.60	121.41	110.24
1	B	48	LYS	CA-C-N	-7.58	113.14	120.34
1	B	48	LYS	C-N-CA	-7.58	113.14	120.34
1	B	403	CYS	N-CA-C	-7.51	99.41	110.52
1	B	26	ASN	N-CA-C	-7.41	102.89	112.23
1	A	298	VAL	CB-CA-C	-7.39	100.17	110.96
1	B	191	GLU	N-CA-C	-7.35	103.27	111.28
1	A	380	THR	N-CA-C	7.32	123.44	111.37
1	A	94	LEU	N-CA-C	7.17	122.03	113.28
1	A	252	GLU	CB-CA-C	7.17	124.43	110.67
1	B	169	SER	N-CA-C	7.15	120.49	111.69
1	A	253	SER	N-CA-C	-7.11	103.53	111.28
1	A	104	ARG	N-CA-C	-7.07	103.58	111.28
1	A	169	SER	N-CA-C	6.91	118.60	111.14
1	B	157	ASN	N-CA-C	6.84	121.78	113.17
1	A	28	LEU	N-CA-C	-6.76	103.91	111.28
1	B	49	GLY	N-CA-C	6.75	120.84	112.14
1	B	376	PRO	N-CA-C	-6.70	98.68	112.47
1	B	296	LEU	N-CA-C	-6.67	100.24	110.32
1	A	345	ALA	N-CA-C	-6.67	104.09	111.36
1	B	249	VAL	N-CA-C	-6.67	102.78	110.05
1	A	287	ARG	N-CA-C	-6.64	101.14	110.50
1	B	393	LYS	N-CA-C	-6.63	100.64	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	VAL	CB-CA-C	-6.60	99.15	110.30
1	A	55	LYS	N-CA-C	6.59	120.19	111.75
1	A	177	ARG	N-CA-C	6.51	119.21	111.33
1	A	229	LEU	N-CA-C	-6.48	100.36	110.14
1	A	290	VAL	CB-CA-C	-6.42	103.36	112.22
1	B	200	SER	N-CA-C	6.36	119.47	110.50
1	B	76	GLU	N-CA-C	6.26	121.39	113.25
1	B	303	ILE	CB-CA-C	-6.22	105.53	111.44
1	B	248	ASN	N-CA-C	6.21	124.02	110.80
1	A	157	ASN	N-CA-C	6.18	120.82	113.16
1	A	390	ARG	N-CA-C	-6.12	105.64	113.23
1	B	116	THR	CA-C-O	-6.09	114.82	119.32
1	B	368	GLY	CA-C-N	6.08	127.84	122.43
1	B	368	GLY	C-N-CA	6.08	127.84	122.43
1	A	170	SER	CA-C-N	6.01	128.58	120.65
1	A	170	SER	C-N-CA	6.01	128.58	120.65
1	A	354	ILE	CB-CA-C	-6.01	103.93	112.22
1	B	124	GLN	CB-CA-C	-6.00	109.63	116.54
1	A	216	TYR	CA-CB-CG	-5.99	103.11	113.90
1	A	272	ASN	N-CA-C	5.98	120.59	112.88
1	B	189	THR	N-CA-C	-5.92	104.91	111.71
1	A	260	ALA	N-CA-C	5.90	120.48	113.28
1	A	200	SER	N-CA-C	5.88	118.34	110.35
1	A	93	VAL	N-CA-C	5.87	116.65	111.90
1	A	113	PRO	N-CA-C	5.78	120.39	111.21
1	B	238	ILE	CB-CA-C	-5.76	102.64	110.42
1	B	254	LEU	CB-CA-C	-5.74	101.09	110.85
1	B	299	LEU	N-CA-C	-5.72	105.40	112.90
1	B	372	ALA	N-CA-C	5.72	120.28	113.12
1	B	348	ALA	N-CA-C	5.71	117.50	111.28
1	B	139	ILE	N-CA-C	-5.69	104.97	110.72
1	B	310	VAL	N-CA-C	-5.67	102.60	109.01
1	A	173	LEU	N-CA-C	-5.67	105.02	111.14
1	A	100	ALA	N-CA-C	5.63	117.42	111.28
1	B	356	LYS	N-CA-C	-5.62	105.24	111.71
1	B	177	ARG	N-CA-C	5.60	118.16	111.71
1	B	364	VAL	N-CA-C	5.58	116.35	108.36
1	A	252	GLU	N-CA-CB	5.58	118.93	110.28
1	B	377	LEU	N-CA-C	5.52	122.57	110.80
1	A	228	ILE	N-CA-C	5.50	116.68	109.58
1	A	160	LYS	N-CA-C	5.50	119.09	112.38
1	A	378	GLY	N-CA-C	5.43	120.73	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ALA	N-CA-C	5.38	117.56	111.11
1	B	246	ARG	CG-CD-NE	5.36	123.80	112.00
1	A	297	PRO	CB-CA-C	-5.36	104.08	111.21
1	B	130	THR	N-CA-C	-5.34	105.63	111.82
1	B	295	ASN	CB-CA-C	-5.32	102.97	112.27
1	A	298	VAL	CA-C-O	-5.31	114.85	120.53
1	B	243	GLU	N-CA-C	5.29	118.99	112.54
1	B	323	ILE	O-C-N	5.28	123.80	120.42
1	A	375	HIS	N-CA-CB	-5.28	102.53	111.30
1	B	70	PHE	N-CA-C	-5.27	105.62	111.36
1	A	356	LYS	CB-CG-CD	5.27	123.41	111.30
1	B	31	LYS	N-CA-C	5.23	116.78	108.67
1	A	129	LEU	N-CA-C	-5.22	105.26	111.69
1	B	84	LEU	N-CA-C	-5.20	106.19	112.54
1	B	389	LEU	N-CA-C	-5.18	99.76	110.80
1	A	76	GLU	N-CA-C	5.16	121.21	109.81
1	A	256	SER	CB-CA-C	-5.16	102.78	110.88
1	B	212	TYR	N-CA-C	-5.16	105.66	111.28
1	A	247	PRO	N-CA-C	-5.12	101.92	111.03
1	B	308	VAL	CG1-CB-CG2	-5.11	99.56	110.80
1	B	69	GLU	N-CA-C	5.10	118.66	112.23
1	B	199	ILE	N-CA-C	-5.09	100.31	107.75
1	B	223	LEU	N-CA-C	5.08	121.62	110.80
1	A	68	ASN	N-CA-C	-5.08	105.64	111.07
1	A	225	GLU	N-CA-C	5.07	117.46	111.33
1	B	249	VAL	CB-CA-C	-5.05	106.03	111.59
1	A	365	ASN	N-CA-CB	-5.05	106.06	111.66
1	A	292	ASN	N-CA-C	-5.04	105.79	111.28
1	B	203	ASP	CB-CA-C	-5.03	102.98	110.88
1	B	72	GLY	N-CA-C	-5.01	106.68	113.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	252	GLU	CA

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	2923	0	2969	115	0
1	B	2951	0	3000	111	0
2	A	8	0	14	0	0
2	B	8	0	14	0	0
3	A	208	0	0	7	0
3	B	240	0	0	16	0
All	All	6338	0	5997	221	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 19.

All (221) 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:207:PHE:HB2	1:B:351:LEU:HD21	1.34	1.08
1:A:354:ILE:HD12	1:A:364:VAL:HG21	1.43	1.00
1:A:188:ILE:HD13	1:A:262:ILE:HD11	1.45	0.95
1:A:201:ARG:HB2	1:A:267:THR:HG22	1.56	0.86
1:B:73:ARG:HH11	1:B:73:ARG:HG3	1.44	0.81
1:B:344:GLU:CD	1:B:369:GLY:HA3	2.06	0.80
1:B:201:ARG:HD3	3:B:615:HOH:O	1.83	0.78
1:A:48:LYS:NZ	1:A:244:GLY:HA2	1.98	0.78
1:B:32:ARG:HD2	3:B:545:HOH:O	1.84	0.76
1:A:354:ILE:CD1	1:A:364:VAL:HG21	2.16	0.74
1:A:191:GLU:HG3	1:A:262:ILE:CD1	2.17	0.74
1:A:121:LEU:CD2	1:B:121:LEU:HD23	2.18	0.73
1:A:81:ASP:OD1	1:A:83:ASN:HB2	1.90	0.72
1:B:226:ASP:HB3	3:B:568:HOH:O	1.91	0.70
1:A:350:ALA:O	1:A:354:ILE:HG12	1.92	0.70
1:B:207:PHE:CB	1:B:351:LEU:HD21	2.17	0.69
1:B:207:PHE:CD2	1:B:351:LEU:HD23	2.28	0.69
1:B:165:LEU:HD22	3:B:716:HOH:O	1.92	0.68
1:B:366:PRO:HA	3:B:742:HOH:O	1.92	0.68
1:A:175:LYS:N	1:A:175:LYS:HD2	2.06	0.68
1:A:252:GLU:HA	1:A:255:SER:OG	1.94	0.67
1:B:394:LYS:N	1:B:394:LYS:HD3	2.08	0.67
1:B:217:LYS:O	1:B:221:GLU:HG3	1.94	0.67
1:A:78:LEU:HD23	1:A:284:LEU:HD21	1.77	0.65
1:A:26:ASN:OD1	1:A:27:SER:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:LEU:HD12	3:A:590:HOH:O	1.97	0.64
1:A:210:ASN:OD1	1:A:214:LYS:HE2	1.97	0.64
1:B:78:LEU:HD21	1:B:284:LEU:HD21	1.81	0.63
1:A:206:GLU:HA	1:A:206:GLU:OE1	1.98	0.63
1:A:311:PRO:HB2	1:A:314:ILE:HD11	1.80	0.62
1:B:210:ASN:ND2	3:B:631:HOH:O	2.31	0.62
1:A:155:MET:O	1:A:159:TYR:HB2	2.00	0.62
1:B:209:ALA:O	1:B:213:GLN:N	2.30	0.62
1:B:203:ASP:O	1:B:206:GLU:HB3	1.99	0.62
1:A:78:LEU:CD2	1:A:284:LEU:HD21	2.29	0.62
1:A:27:SER:O	1:A:32:ARG:NH2	2.30	0.62
1:A:46:ILE:HG12	3:A:628:HOH:O	1.98	0.62
1:A:155:MET:HG3	1:A:277:SER:O	2.00	0.61
1:A:192:ASN:O	1:A:196:ASN:HB2	2.00	0.61
1:B:222:GLY:O	1:B:225:GLU:HB2	2.00	0.61
1:A:27:SER:HA	1:A:30:GLU:HG3	1.82	0.61
1:B:74:PHE:HB2	1:B:79:ARG:HG2	1.83	0.60
1:A:377:LEU:HD13	3:A:685:HOH:O	2.00	0.60
1:B:390:ARG:H	1:B:390:ARG:HD2	1.65	0.60
1:B:232:LYS:NZ	1:B:236:GLY:O	2.30	0.59
1:B:25:LYS:O	1:B:29:LEU:HD23	2.02	0.59
1:A:210:ASN:O	1:A:214:LYS:HG3	2.03	0.59
1:A:300:GLY:HA2	1:A:417:GLU:HG3	1.85	0.59
1:B:314:ILE:O	1:B:317:VAL:HG22	2.03	0.59
1:B:390:ARG:HD2	1:B:390:ARG:N	2.17	0.59
1:B:63:LEU:HD11	1:B:150:LEU:HD13	1.86	0.58
1:A:188:ILE:HD13	1:A:262:ILE:CD1	2.29	0.57
1:A:75:PRO:C	1:A:77:PRO:HD2	2.30	0.57
1:B:252:GLU:N	3:B:715:HOH:O	2.37	0.57
1:B:27:SER:O	1:B:30:GLU:HB3	2.05	0.57
1:A:188:ILE:CD1	1:A:262:ILE:HD11	2.27	0.56
1:A:344:GLU:CD	1:A:369:GLY:HA3	2.31	0.56
1:A:121:LEU:HD23	1:B:121:LEU:HD23	1.88	0.56
1:B:176:ASN:O	1:B:180:LYS:HG2	2.06	0.56
1:A:218:ALA:HA	1:A:223:LEU:HD12	1.87	0.56
1:A:25:LYS:O	1:A:28:LEU:HB2	2.06	0.56
1:A:324:PRO:HD3	1:A:357:LEU:HD21	1.88	0.56
1:B:163:ASN:OD1	1:B:164:PRO:HD2	2.06	0.55
1:B:251:ALA:O	1:B:254:LEU:HB2	2.06	0.55
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.70	0.55
1:A:232:LYS:HG3	1:A:237:SER:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:SER:O	1:B:32:ARG:NH1	2.37	0.55
1:B:73:ARG:HG3	1:B:73:ARG:NH1	2.18	0.55
1:B:215:ALA:O	1:B:219:LYS:HB2	2.06	0.55
1:B:223:LEU:HB3	1:B:367:ARG:NH1	2.23	0.55
1:B:383:ARG:HD2	1:B:383:ARG:C	2.32	0.55
1:A:252:GLU:HB3	1:A:255:SER:OG	2.06	0.54
1:B:207:PHE:HB2	1:B:351:LEU:CD2	2.24	0.54
1:B:323:ILE:HB	1:B:324:PRO:HD3	1.89	0.54
1:A:73:ARG:O	1:A:73:ARG:HG3	2.08	0.54
1:A:261:PHE:C	1:A:262:ILE:HG13	2.33	0.54
1:B:344:GLU:OE2	1:B:369:GLY:HA3	2.07	0.54
1:B:335:GLN:HB2	3:B:612:HOH:O	2.06	0.53
1:A:73:ARG:NH1	1:A:226:ASP:O	2.35	0.53
1:A:250:THR:HG1	1:A:253:SER:CB	2.21	0.53
1:A:191:GLU:OE2	1:A:268:THR:HB	2.08	0.53
1:B:37:VAL:HB	1:B:298:VAL:HG13	1.91	0.53
1:A:233:LEU:HD22	1:A:233:LEU:N	2.24	0.52
1:A:289:SER:O	1:A:293:GLN:NE2	2.42	0.52
1:A:308:VAL:CG1	1:A:325:LYS:HD2	2.39	0.52
1:A:339:ILE:CG1	1:A:392:LEU:HD23	2.40	0.52
1:B:248:ASN:HA	3:B:671:HOH:O	2.09	0.52
1:A:48:LYS:HZ2	1:A:244:GLY:HA2	1.74	0.51
1:A:48:LYS:HZ3	1:A:244:GLY:HA2	1.74	0.51
1:A:339:ILE:HG12	1:A:392:LEU:HD23	1.91	0.51
1:A:79:ARG:HH11	1:A:79:ARG:CG	2.23	0.50
1:A:308:VAL:HG13	1:A:325:LYS:HD3	1.93	0.50
1:A:32:ARG:NH1	3:A:597:HOH:O	2.45	0.50
1:B:73:ARG:HH11	1:B:73:ARG:CG	2.20	0.50
1:B:83:ASN:ND2	1:B:115:SER:OG	2.41	0.50
1:A:313:GLU:HG2	1:A:314:ILE:HG13	1.93	0.50
1:B:213:GLN:NE2	1:B:249:VAL:O	2.41	0.50
1:B:233:LEU:HB3	1:B:234:PRO:CD	2.41	0.50
1:A:201:ARG:HB2	1:A:267:THR:CG2	2.34	0.49
1:A:79:ARG:HB3	1:A:79:ARG:CZ	2.42	0.49
1:A:178:GLU:HA	1:A:178:GLU:OE1	2.12	0.49
1:A:261:PHE:HB2	1:A:262:ILE:HD12	1.93	0.49
1:A:325:LYS:HE3	3:A:598:HOH:O	2.12	0.49
1:B:81:ASP:OD1	1:B:83:ASN:HB2	2.12	0.49
1:A:250:THR:N	1:A:253:SER:OG	2.44	0.49
1:A:303:ILE:HD11	1:A:415:ILE:HD12	1.94	0.49
1:A:308:VAL:HG13	1:A:325:LYS:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ALA:HB2	1:B:243:GLU:OE2	2.13	0.49
1:B:390:ARG:H	1:B:390:ARG:CD	2.23	0.49
1:B:213:GLN:HG3	3:B:729:HOH:O	2.13	0.48
1:A:114:TYR:O	1:B:309:GLY:HA3	2.12	0.48
1:B:264:ASP:O	1:B:265:ARG:HD3	2.12	0.48
1:A:191:GLU:HG3	1:A:262:ILE:HD13	1.94	0.48
1:A:76:GLU:OE2	1:A:79:ARG:NE	2.43	0.48
1:A:404:ILE:HB	1:A:408:MET:HB2	1.95	0.48
1:A:234:PRO:C	1:A:236:GLY:H	2.22	0.48
1:A:309:GLY:HA3	1:B:114:TYR:O	2.14	0.48
1:A:200:SER:O	1:A:204:GLN:HG3	2.14	0.48
1:B:251:ALA:N	3:B:715:HOH:O	2.47	0.48
1:A:176:ASN:HB3	1:A:179:ALA:HB3	1.95	0.48
1:A:344:GLU:OE2	1:A:369:GLY:HA3	2.14	0.48
1:B:338:ASP:O	1:B:339:ILE:HG13	2.13	0.48
1:A:201:ARG:HE	1:A:205:ASP:CG	2.22	0.47
1:B:89:ALA:HB1	1:B:121:LEU:HD11	1.95	0.47
1:B:178:GLU:HA	1:B:178:GLU:OE1	2.15	0.47
1:A:174:GLN:C	1:A:175:LYS:HD2	2.40	0.47
1:A:181:LYS:C	1:A:183:LEU:H	2.23	0.47
1:A:237:SER:O	1:A:238:ILE:HG13	2.14	0.47
1:B:124:GLN:HB2	1:B:404:ILE:HG23	1.97	0.47
1:B:251:ALA:O	1:B:254:LEU:N	2.44	0.47
1:A:311:PRO:CB	1:A:314:ILE:HD11	2.45	0.47
1:B:249:VAL:HG12	1:B:250:THR:N	2.29	0.47
1:A:180:LYS:NZ	3:A:687:HOH:O	2.48	0.47
1:B:76:GLU:HG3	3:B:708:HOH:O	2.15	0.46
1:B:235:ASP:OD1	1:B:237:SER:N	2.31	0.46
1:B:400:VAL:O	1:B:411:ALA:HA	2.15	0.46
1:A:320:ALA:O	1:A:324:PRO:HG2	2.16	0.46
1:A:42:ASN:HD21	1:A:73:ARG:NH1	2.13	0.46
1:A:354:ILE:HD11	1:A:364:VAL:HG11	1.98	0.46
1:A:261:PHE:O	1:A:262:ILE:HG13	2.16	0.46
1:B:361:LEU:CD2	1:B:361:LEU:H	2.29	0.46
1:A:258:ARG:O	1:A:269:THR:HB	2.15	0.45
1:A:252:GLU:O	1:A:255:SER:OG	2.30	0.45
1:B:232:LYS:HE3	1:B:236:GLY:HA2	1.98	0.45
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.30	0.45
1:A:216:TYR:CE2	1:A:247:PRO:HB3	2.50	0.45
1:A:76:GLU:N	1:A:77:PRO:CD	2.80	0.45
1:A:233:LEU:N	1:A:233:LEU:CD2	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLU:OE1	1:B:76:GLU:HA	2.16	0.45
1:B:389:LEU:O	1:B:391:GLU:N	2.50	0.45
1:A:315:MET:HE1	1:A:403:CYS:SG	2.57	0.45
1:B:73:ARG:NH1	1:B:73:ARG:CG	2.80	0.45
1:B:178:GLU:HA	1:B:181:LYS:HD2	1.99	0.45
1:B:75:PRO:HG2	1:B:296:LEU:HD22	1.99	0.45
1:A:171:GLU:HA	1:A:171:GLU:OE1	2.17	0.44
1:B:192:ASN:O	1:B:196:ASN:HB2	2.17	0.44
1:B:361:LEU:CD2	1:B:361:LEU:N	2.79	0.44
1:A:406:THR:HB	1:B:104:ARG:HG2	1.98	0.44
1:B:53:ALA:H	1:B:243:GLU:CD	2.24	0.44
1:B:365:ASN:N	1:B:366:PRO:CD	2.80	0.44
1:B:403:CYS:C	1:B:404:ILE:HG13	2.42	0.44
1:A:183:LEU:O	1:A:185:PRO:HD3	2.18	0.44
1:B:249:VAL:CG1	1:B:250:THR:N	2.80	0.44
1:A:311:PRO:CG	1:A:314:ILE:HD11	2.48	0.44
1:A:383:ARG:HD2	1:A:383:ARG:C	2.42	0.44
1:B:339:ILE:HD12	1:B:392:LEU:HD23	1.98	0.44
1:B:344:GLU:OE1	1:B:369:GLY:HA3	2.17	0.44
1:B:361:LEU:N	1:B:361:LEU:HD22	2.33	0.44
1:B:210:ASN:OD1	1:B:214:LYS:HE2	2.18	0.44
1:A:340:PHE:CE2	1:A:359:ILE:HG12	2.52	0.44
1:A:178:GLU:HA	1:A:181:LYS:HD2	2.00	0.44
1:B:394:LYS:O	1:B:395:ASP:HB2	2.18	0.44
1:B:343:ASN:HD21	1:B:370:ALA:HB2	1.83	0.43
1:A:341:GLU:OE2	1:A:391:GLU:OE1	2.37	0.43
1:B:255:SER:HB3	3:B:650:HOH:O	2.18	0.43
1:A:198:LYS:HA	1:A:198:LYS:HD2	1.71	0.43
1:B:390:ARG:N	1:B:390:ARG:CD	2.81	0.43
1:A:67:LEU:O	1:A:71:ILE:HG13	2.19	0.43
1:A:323:ILE:HB	1:A:324:PRO:HD3	2.00	0.43
1:A:168:ILE:HG13	1:A:183:LEU:HD21	2.01	0.43
1:A:361:LEU:HD13	1:A:361:LEU:HA	1.35	0.43
1:A:171:GLU:O	1:A:174:GLN:HB2	2.19	0.43
1:A:324:PRO:HG3	1:A:357:LEU:CD2	2.49	0.43
1:B:82:LEU:HD23	1:B:82:LEU:HA	1.78	0.43
1:B:200:SER:O	1:B:204:GLN:HG3	2.19	0.43
1:A:79:ARG:CG	1:A:79:ARG:NH1	2.80	0.43
1:A:299:LEU:HD23	1:A:299:LEU:N	2.34	0.43
1:B:257:ILE:HG22	1:B:258:ARG:N	2.33	0.42
1:A:186:MET:HG3	3:A:645:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:GLU:HB2	1:B:223:LEU:HG	2.01	0.42
1:B:233:LEU:HB3	1:B:234:PRO:HD3	2.01	0.42
1:B:257:ILE:CG2	1:B:258:ARG:N	2.82	0.42
1:A:307:THR:HG22	1:A:410:ALA:HB2	2.01	0.42
1:A:227:GLU:HB3	1:A:390:ARG:HD3	2.01	0.42
1:A:48:LYS:HB2	1:A:48:LYS:HE2	1.50	0.42
1:B:226:ASP:N	3:B:618:HOH:O	2.35	0.42
1:B:319:PRO:HD2	1:B:353:CYS:SG	2.60	0.42
1:B:359:ILE:HG22	1:B:360:ASP:N	2.34	0.42
1:B:200:SER:O	1:B:203:ASP:HB2	2.19	0.42
1:B:394:LYS:HD2	1:B:417:GLU:O	2.20	0.42
1:B:359:ILE:CG2	1:B:360:ASP:N	2.81	0.41
1:A:32:ARG:O	1:A:288:ARG:HD2	2.20	0.41
1:B:207:PHE:CD2	1:B:351:LEU:CD2	3.00	0.41
1:B:223:LEU:O	1:B:367:ARG:NH1	2.52	0.41
1:B:202:LYS:H	1:B:202:LYS:HG2	1.26	0.41
1:B:124:GLN:HG3	1:B:405:GLY:O	2.21	0.41
1:B:263:LYS:H	1:B:263:LYS:HG2	1.70	0.41
1:B:83:ASN:ND2	3:B:613:HOH:O	2.50	0.41
1:B:235:ASP:OD1	1:B:237:SER:OG	2.37	0.41
1:A:163:ASN:HA	1:A:164:PRO:HD2	1.48	0.41
1:B:287:ARG:NH1	3:B:555:HOH:O	2.52	0.41
1:B:215:ALA:O	1:B:219:LYS:N	2.49	0.40
1:B:301:ARG:HD3	1:B:417:GLU:OE2	2.21	0.40
1:A:250:THR:O	1:A:253:SER:OG	2.30	0.40
1:A:324:PRO:HG3	1:A:357:LEU:HD21	2.03	0.40
1:B:124:GLN:HB2	1:B:404:ILE:CG2	2.51	0.40
1:A:79:ARG:CZ	1:A:79:ARG:CB	3.00	0.40
1:B:118:PHE:CD1	1:B:118:PHE:C	2.99	0.40
1:B:337:ILE:HB	1:B:340:PHE:CZ	2.56	0.40
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.86	0.40
1:B:305:PHE:CD1	1:B:305:PHE:C	3.00	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	386/393 (98%)	366 (95%)	18 (5%)	2 (0%)	24	14
1	B	391/393 (100%)	364 (93%)	23 (6%)	4 (1%)	12	4
All	All	777/786 (99%)	730 (94%)	41 (5%)	6 (1%)	16	6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	LEU
1	B	377	LEU
1	B	390	ARG
1	B	223	LEU
1	B	251	ALA
1	A	235	ASP

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	311/314 (99%)	274 (88%)	37 (12%)	5	1
1	B	314/314 (100%)	281 (90%)	33 (10%)	6	2
All	All	625/628 (100%)	555 (89%)	70 (11%)	6	1

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	28	LEU
1	A	29	LEU
1	A	48	LYS
1	A	73	ARG
1	A	76	GLU

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Mol	Chain	Res	Type
1	A	78	LEU
1	A	160	LYS
1	A	170	SER
1	A	172	GLU
1	A	177	ARG
1	A	196	ASN
1	A	206	GLU
1	A	217	LYS
1	A	219	LYS
1	A	221	GLU
1	A	232	LYS
1	A	243	GLU
1	A	246	ARG
1	A	252	GLU
1	A	256	SER
1	A	257	ILE
1	A	258	ARG
1	A	262	ILE
1	A	267	THR
1	A	280	VAL
1	A	293	GLN
1	A	299	LEU
1	A	308	VAL
1	A	314	ILE
1	A	333	GLN
1	A	335	GLN
1	A	349	GLN
1	A	356	LYS
1	A	361	LEU
1	A	362	ASN
1	A	388	ILE
1	B	26	ASN
1	B	28	LEU
1	B	48	LYS
1	B	79	ARG
1	B	83	ASN
1	B	110	SER
1	B	130	THR
1	B	165	LEU
1	B	169	SER
1	B	171	GLU
1	B	180	LYS

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Mol	Chain	Res	Type
1	B	202	LYS
1	B	206	GLU
1	B	210	ASN
1	B	219	LYS
1	B	232	LYS
1	B	233	LEU
1	B	246	ARG
1	B	248	ASN
1	B	250	THR
1	B	252	GLU
1	B	256	SER
1	B	277	SER
1	B	324	PRO
1	B	333	GLN
1	B	335	GLN
1	B	349	GLN
1	B	365	ASN
1	B	377	LEU
1	B	389	LEU
1	B	394	LYS
1	B	399	VAL
1	B	416	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	157	ASN
1	A	292	ASN
1	A	293	GLN
1	B	68	ASN
1	B	83	ASN
1	B	95	ASN
1	B	124	GLN
1	B	292	ASN
1	B	306	GLN
1	B	343	ASN
1	B	355	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	MRD	A	501	-	7,7,7	0.56	0	9,10,10	2.32	2 (22%)
2	MRD	B	502	-	7,7,7	0.49	0	9,10,10	1.54	2 (22%)

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	MRD	A	501	-	-	1/5/5/5	-
2	MRD	B	502	-	-	1/5/5/5	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MRD	CM-C2-C1	-5.11	99.19	110.63
2	A	501	MRD	O2-C2-C1	4.09	120.74	107.99
2	B	502	MRD	CM-C2-C1	-2.93	104.05	110.63
2	B	502	MRD	O4-C4-C3	-2.53	101.27	111.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	MRD	O2-C2-C3-C4
2	B	502	MRD	CM-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	390/393 (99%)	-0.52	3 (0%) 82 83	7, 22, 56, 92	0
1	B	393/393 (100%)	-0.51	4 (1%) 79 80	6, 21, 51, 84	0
All	All	783/786 (99%)	-0.52	7 (0%) 81 81	6, 22, 53, 92	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	ILE	3.1
1	A	26	ASN	2.4
1	B	220	ASN	2.4
1	B	216	TYR	2.3
1	B	26	ASN	2.3
1	B	254	LEU	2.1
1	A	293	GLN	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	MRD	A	501	8/8	0.90	0.08	28,34,43,44	0
2	MRD	B	502	8/8	0.95	0.06	21,24,30,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.