



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:30 PM UTC

PDB ID : 4CVW / pdb_00004cvw
Title : Structure of the barley limit dextrinase-limit dextrinase inhibitor complex
Authors : Moeller, M.S.; Vester-Christensen, M.B.; Jensen, J.M.; Abou Hachem, M.;
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Deposited on : 2014-03-31
Resolution : 2.67 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
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

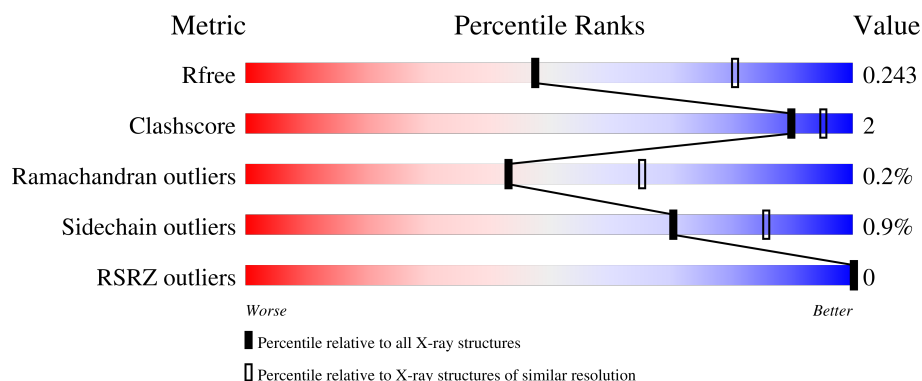
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	884	 92% 6% •
1	B	884	 93% 5% •
2	C	120	 78% 6% 16%
2	D	120	 81% • 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15152 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 LIMIT DEXTRINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	874	Total	C	N	O	S	0	0	0
			6766	4277	1162	1297	30			
1	B	871	Total	C	N	O	S	0	1	0
			6740	4263	1154	1292	31			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ARG	LYS	engineered mutation	UNP O48541
A	484	MET	-	insertion	UNP O48541
A	485	ARG	VAL	engineered mutation	UNP O48541
A	486	ALA	THR	engineered mutation	UNP O48541
B	82	ARG	LYS	engineered mutation	UNP O48541
B	484	MET	-	insertion	UNP O48541
B	485	ARG	VAL	engineered mutation	UNP O48541
B	486	ALA	THR	engineered mutation	UNP O48541

- Molecule 2 is a protein called LIMIT DEXTRINASE INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	101	Total	C	N	O	S	0	0	0
			770	468	152	139	11			
2	D	102	Total	C	N	O	S	0	0	0
			774	471	153	139	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	115	HIS	-	expression tag	UNP Q2V8X0
C	116	HIS	-	expression tag	UNP Q2V8X0
C	117	HIS	-	expression tag	UNP Q2V8X0
C	118	HIS	-	expression tag	UNP Q2V8X0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	119	HIS	-	expression tag	UNP Q2V8X0
C	120	HIS	-	expression tag	UNP Q2V8X0
D	115	HIS	-	expression tag	UNP Q2V8X0
D	116	HIS	-	expression tag	UNP Q2V8X0
D	117	HIS	-	expression tag	UNP Q2V8X0
D	118	HIS	-	expression tag	UNP Q2V8X0
D	119	HIS	-	expression tag	UNP Q2V8X0
D	120	HIS	-	expression tag	UNP Q2V8X0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0
3	B	2	Total Ca 2 2	0	0

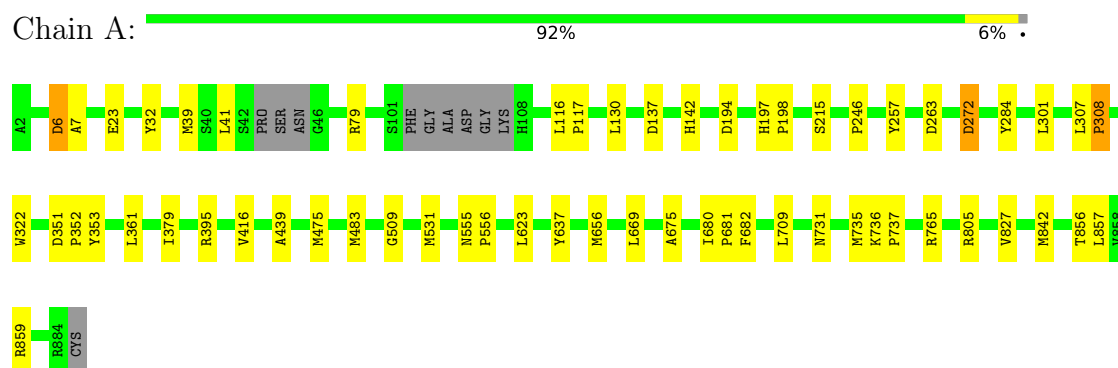
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	57	Total O 57 57	0	0
4	B	39	Total O 39 39	0	0
4	D	2	Total O 2 2	0	0

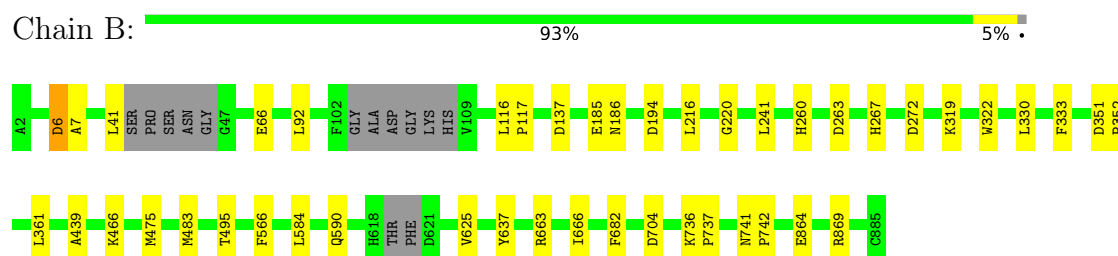
3 Residue-property plots

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.

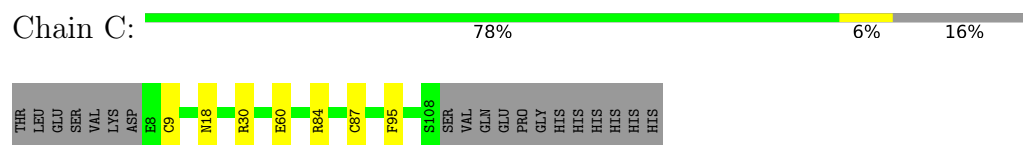
• Molecule 1: LIMIT DEXTRINASE



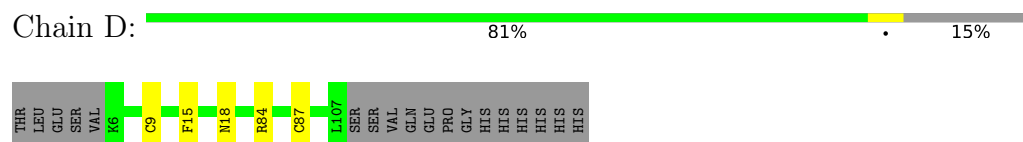
• Molecule 1: LIMIT DEXTRINASE



• Molecule 2: LIMIT DEXTRINASE INHIBITOR



• Molecule 2: LIMIT DEXTRINASE INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	166.98Å 168.61Å 157.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	157.76 – 2.67 118.64 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.3 (157.76-2.67) 96.4 (118.64-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.255 , 0.293 0.211 , 0.243	Depositor DCC
R_{free} test set	3083 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.448 for -k,-h,-l	Xtriage
Reported twinning fraction	0.559 for H, K, L 0.441 for K, H, -L	Depositor
Outliers	3 of 60738 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15152	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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:
CA

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	0.43	0/6934	0.76	3/9431 (0.0%)
1	B	0.43	0/6906	0.75	0/9394
2	C	0.45	0/783	0.82	2/1057 (0.2%)
2	D	0.45	0/787	0.81	2/1063 (0.2%)
All	All	0.43	0/15410	0.76	7/20945 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	18	ASN	CA-C-N	5.44	124.90	119.24
2	D	18	ASN	C-N-CA	5.44	124.90	119.24
1	A	623	LEU	N-CA-C	5.43	118.01	110.20
1	A	353	TYR	N-CA-C	5.12	117.32	109.07
2	C	18	ASN	CA-C-N	5.11	124.55	119.24
2	C	18	ASN	C-N-CA	5.11	124.55	119.24
1	A	509	GLY	N-CA-C	5.05	117.94	110.42

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	6766	0	6493	28	0
1	B	6740	0	6462	21	0
2	C	770	0	751	3	0
2	D	774	0	750	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	57	0	0	0	0
4	B	39	0	0	0	0
4	D	2	0	0	0	0
All	All	15152	0	14456	54	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 2.

All (54) 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:116:LEU:N	1:B:117:PRO:HD2	1.98	0.79
1:B:475:MET:HE3	1:B:483:MET:HE2	1.68	0.76
1:A:475:MET:HE2	1:A:531:MET:HG3	1.79	0.64
1:B:322:TRP:CD2	1:B:352:PRO:HB3	2.39	0.58
1:A:32:TYR:HB3	1:A:39:MET:HE1	1.85	0.57
1:A:23:GLU:HA	1:A:79:ARG:HE	1.69	0.57
1:B:6:ASP:OD1	1:B:7:ALA:N	2.38	0.56
1:B:116:LEU:N	1:B:117:PRO:CD	2.68	0.55
1:A:6:ASP:OD1	1:A:7:ALA:N	2.39	0.55
1:A:805:ARG:NH1	1:A:842:MET:HE3	2.22	0.55
1:A:116:LEU:N	1:A:117:PRO:CD	2.73	0.51
2:C:84:ARG:HB2	2:C:87:CYS:HB3	1.93	0.50
1:A:637:TYR:HB3	1:A:682:PHE:HB3	1.94	0.49
1:A:736:LYS:HB3	1:A:737:PRO:HD3	1.94	0.49
2:D:84:ARG:HB2	2:D:87:CYS:HB3	1.96	0.47
1:A:669:LEU:HD13	1:A:827:VAL:HG12	1.96	0.47
1:A:322:TRP:CD2	1:A:352:PRO:HB3	2.50	0.47
1:B:663:ARG:HA	1:B:666:ILE:HD12	1.98	0.46
1:A:130:LEU:HA	1:A:142:HIS:HB2	1.98	0.46
1:A:856:THR:HA	1:A:859:ARG:HD3	1.97	0.46
1:B:267:HIS:CE1	1:B:704:ASP:HB3	2.51	0.46
1:B:637:TYR:HB3	1:B:682:PHE:HB3	1.97	0.46
1:B:185:GLU:O	1:B:186:ASN:HB2	2.15	0.45
1:B:736:LYS:HB3	1:B:737:PRO:HD3	1.97	0.45
1:A:215:SER:HB2	1:A:379:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:TYR:HB2	1:A:301:LEU:HD11	1.99	0.45
2:D:9:CYS:HB3	2:D:15:PHE:HE2	1.82	0.45
1:B:241:LEU:HD23	1:B:466:LYS:HD2	1.98	0.45
1:A:675:ALA:O	1:A:765:ARG:HD2	2.17	0.45
1:A:272:ASP:HB3	1:A:284:TYR:OH	2.16	0.44
1:B:330:LEU:HA	1:B:333:PHE:CD2	2.52	0.44
1:A:361:LEU:HD21	1:A:416:VAL:HG11	1.99	0.44
1:A:475:MET:HE3	1:A:483:MET:HE2	2.00	0.43
1:B:216:LEU:HB3	1:B:220:GLY:HA2	2.00	0.43
1:A:656:MET:HE1	1:A:737:PRO:HB2	2.00	0.43
1:A:246:PRO:HG2	1:A:395:ARG:HG3	2.01	0.42
1:A:197:HIS:HA	1:A:198:PRO:HD3	1.89	0.42
1:A:263:ASP:HB3	1:A:709:LEU:HD12	1.99	0.42
1:B:864:GLU:HB2	1:B:869:ARG:HB3	2.02	0.42
1:A:351:ASP:HB2	1:A:352:PRO:HD2	2.00	0.42
1:B:351:ASP:HB2	1:B:352:PRO:HD2	2.00	0.42
1:A:680:ILE:HA	1:A:681:PRO:HD3	1.92	0.42
2:C:9:CYS:HB2	2:C:60:GLU:HG2	2.01	0.42
2:C:30:ARG:HG2	2:C:95:PHE:CZ	2.55	0.42
1:B:566:PHE:HB3	1:B:584:LEU:HD22	2.02	0.41
1:A:731:ASN:CB	1:A:735:MET:HE3	2.51	0.41
1:A:307:LEU:HB3	1:A:308:PRO:HD2	2.03	0.41
1:B:260:HIS:HB3	1:B:263:ASP:HB2	2.01	0.41
1:B:216:LEU:HD11	1:B:361:LEU:HD12	2.02	0.41
1:B:741:ASN:HA	1:B:742:PRO:HD3	1.85	0.41
1:A:555:ASN:HA	1:A:556:PRO:HD3	1.92	0.40
1:A:805:ARG:HH12	1:A:842:MET:HE3	1.85	0.40
1:B:319:LYS:HG2	1:B:322:TRP:CH2	2.57	0.40
1:B:590:GLN:HG2	1:B:625:VAL:HG21	2.02	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	868/884 (98%)	833 (96%)	33 (4%)	2 (0%)	43	65
1	B	864/884 (98%)	830 (96%)	33 (4%)	1 (0%)	48	71
2	C	99/120 (82%)	94 (95%)	5 (5%)	0	100	100
2	D	100/120 (83%)	94 (94%)	6 (6%)	0	100	100
All	All	1931/2008 (96%)	1851 (96%)	77 (4%)	3 (0%)	43	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	ALA
1	B	439	ALA
1	A	308	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	726/742 (98%)	720 (99%)	6 (1%)	73	87
1	B	723/742 (97%)	715 (99%)	8 (1%)	65	83
2	C	83/103 (81%)	83 (100%)	0	100	100
2	D	82/103 (80%)	82 (100%)	0	100	100
All	All	1614/1690 (96%)	1600 (99%)	14 (1%)	70	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	41	LEU
1	A	137	ASP
1	A	194	ASP
1	A	272	ASP
1	A	857	LEU
1	B	6	ASP
1	B	41	LEU

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Mol	Chain	Res	Type
1	B	66	GLU
1	B	92	LEU
1	B	137	ASP
1	B	194	ASP
1	B	272	ASP
1	B	495	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	197	HIS
1	A	202	GLN
1	A	260	HIS
1	A	348	GLN
1	A	390	ASN
1	A	433	GLN
1	A	498	HIS
1	A	592	GLN
1	A	643	ASN
1	A	731	ASN
1	B	230	ASN
1	B	348	GLN
1	B	384	GLN
1	B	390	ASN
1	B	562	ASN
2	C	92	GLN
2	D	56	HIS
2	D	92	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

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	874/884 (98%)	-1.63	0 100 100	11, 23, 37, 41	0
1	B	871/884 (98%)	-1.64	0 100 100	11, 23, 37, 41	1 (0%)
2	C	101/120 (84%)	-1.53	0 100 100	31, 38, 42, 42	0
2	D	102/120 (85%)	-1.52	0 100 100	31, 38, 41, 42	0
All	All	1948/2008 (97%)	-1.62	0 100 100	11, 24, 39, 42	1 (0%)

There are no RSRZ outliers to report.

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	CA	A	1885	1/1	0.99	0.02	15,15,15,15	0
3	CA	B	1887	1/1	0.99	0.02	14,14,14,14	0
3	CA	B	1886	1/1	1.00	0.02	14,14,14,14	0
3	CA	A	1886	1/1	1.00	0.01	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.