



wwPDB X-ray Structure Validation Summary Report

Feb 17, 2024 – 04:49 PM EST

PDB ID : 3TEN
Title : Holo form of carbon disulfide hydrolase
Authors : Smeulders, M.J.; Barends, T.R.M.B.; Pol, A.; Scherer, A.; Zandvoort, M.H.;
Udvarhelyi, A.; Khadem, A.; Menzel, A.; Hermans, J.; Shoeman, R.L.; Wes-
sels, H.J.C.T.; van den Heuvel, L.P.; Russ, L.; Schlichting, I.; Jetten, M.S.M.;
Op den Camp, H.J.M.
Deposited on : 2011-08-15
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

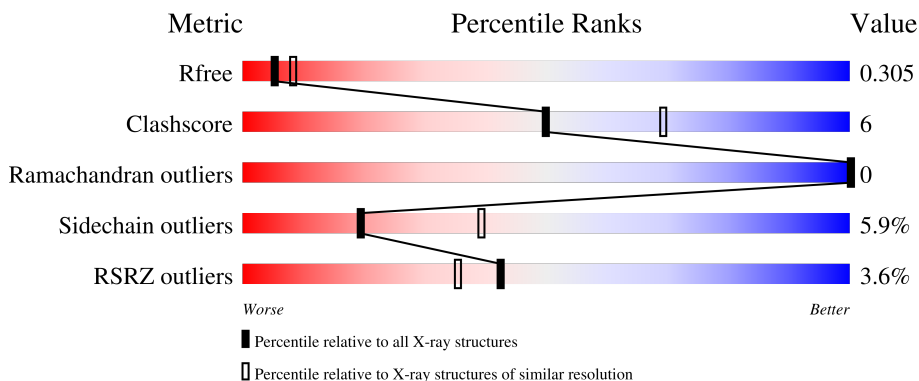
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



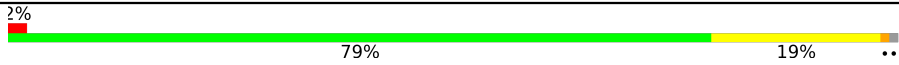

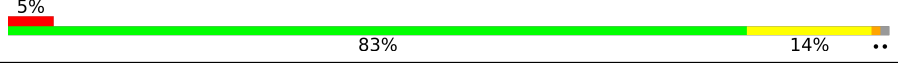
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	204	 2% 84% 14% ..
1	B	204	 2% 85% 13% ..
1	C	204	 6% 84% 14% ..
1	D	204	 4% 80% 16% ..
1	E	204	 2% 83% 14% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	204	 2% 79% 19% ..
1	G	204	 4% 84% 13% ..
1	H	204	 5% 83% 14% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13295 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 CS2 hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	1637	1045	282	305	5	0	0	0
1	B	201	1637	1045	282	305	5	0	0	0
1	C	201	1637	1045	282	305	5	0	0	0
1	D	201	1637	1045	282	305	5	0	0	0
1	E	201	1637	1045	282	305	5	0	0	0
1	F	201	1637	1045	282	305	5	0	0	0
1	G	201	1637	1045	282	305	5	0	0	0
1	H	201	1637	1045	282	305	5	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0

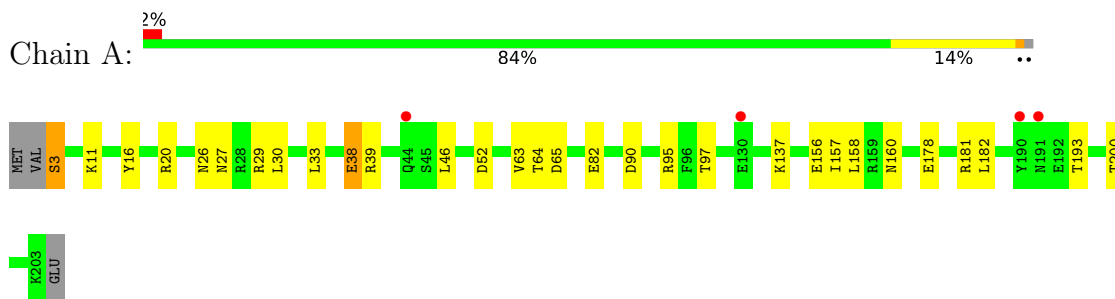
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0
3	B	22	Total 22	O 22	0	0
3	C	26	Total 26	O 26	0	0
3	D	25	Total 25	O 25	0	0
3	E	27	Total 27	O 27	0	0
3	F	25	Total 25	O 25	0	0
3	G	24	Total 24	O 24	0	0
3	H	20	Total 20	O 20	0	0

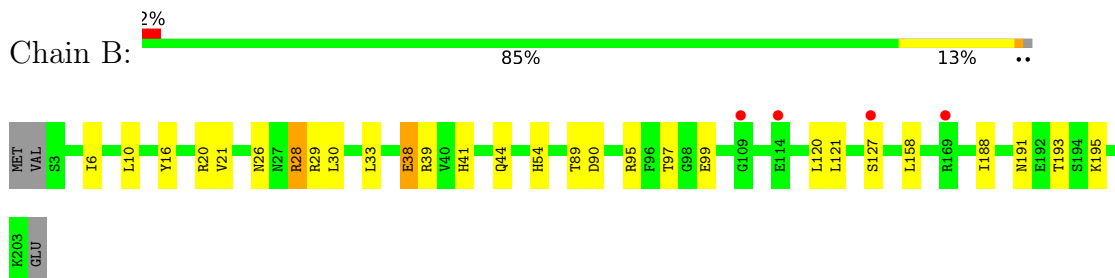
3 Residue-property plots [i](#)

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.

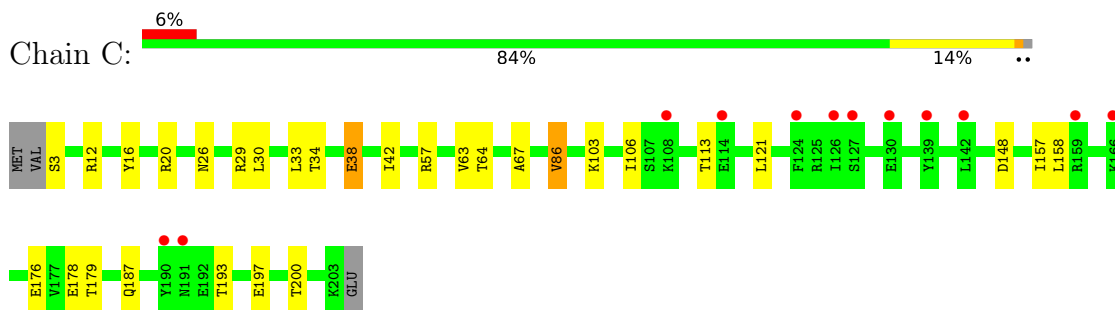
- Molecule 1: CS2 hydrolase



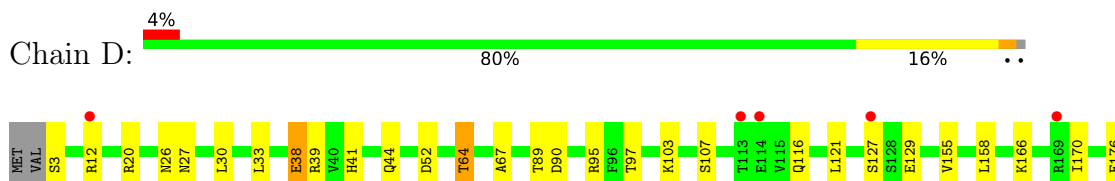
- Molecule 1: CS2 hydrolase



- Molecule 1: CS2 hydrolase

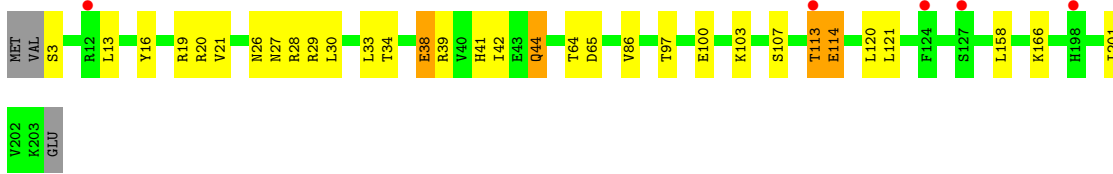
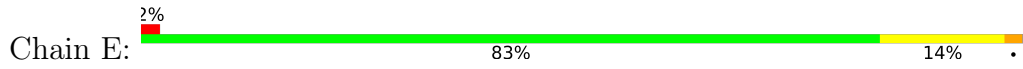


- Molecule 1: CS2 hydrolase

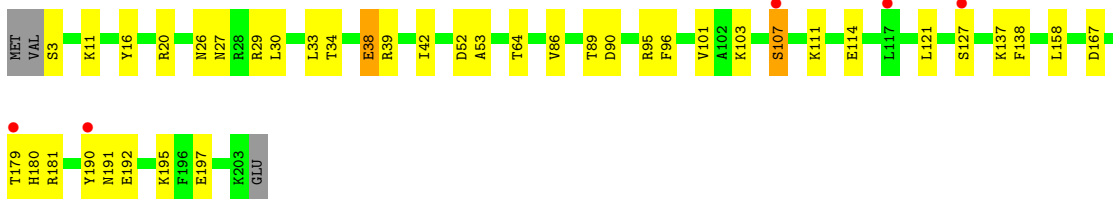
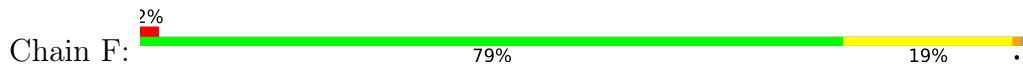




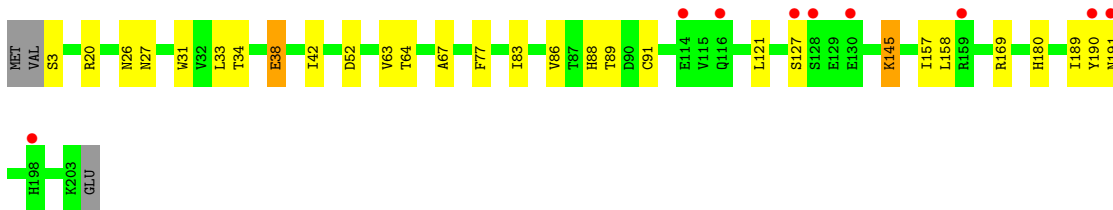
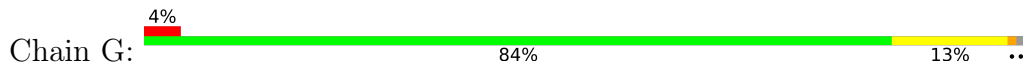
- Molecule 1: CS2 hydrolase



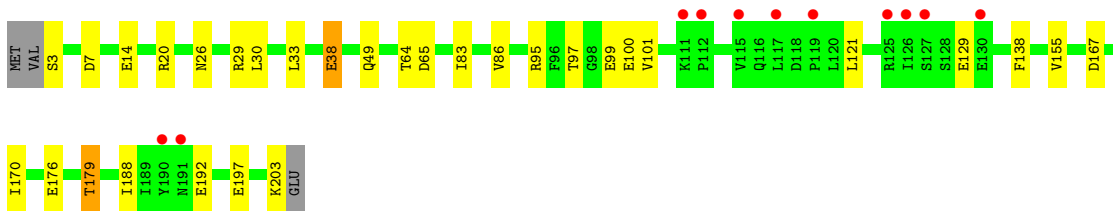
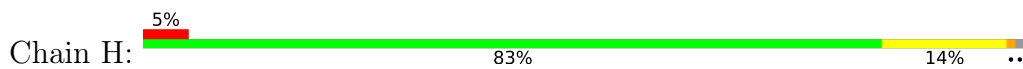
- Molecule 1: CS2 hydrolase



- Molecule 1: CS2 hydrolase



- Molecule 1: CS2 hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	204.95Å 113.24Å 87.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 75.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-2.60) 100.0 (75.98-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.62Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.266 , 0.299 0.270 , 0.305	Depositor DCC
R_{free} test set	3320 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtrriage
Anisotropy	0.641	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13295	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.86 % 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 2.5730e-05. 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:
ZN

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	0.44	0/1672	0.57	0/2260
1	B	0.43	0/1672	0.62	0/2260
1	C	0.44	0/1672	0.58	0/2260
1	D	0.41	0/1672	0.61	0/2260
1	E	0.41	0/1672	0.58	0/2260
1	F	0.40	0/1672	0.58	0/2260
1	G	0.42	0/1672	0.58	0/2260
1	H	0.42	0/1672	0.59	0/2260
All	All	0.42	0/13376	0.59	0/18080

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	28	ARG	Peptide

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	1637	0	1638	30	0
1	B	1637	0	1638	22	0
1	C	1637	0	1638	20	0
1	D	1637	0	1638	27	0
1	E	1637	0	1638	26	0
1	F	1637	0	1638	32	0
1	G	1637	0	1638	21	0
1	H	1637	0	1638	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	22	0	0	3	0
3	B	22	0	0	4	0
3	C	26	0	0	5	0
3	D	25	0	0	6	0
3	E	27	0	0	5	0
3	F	25	0	0	3	0
3	G	24	0	0	5	0
3	H	20	0	0	4	0
All	All	13295	0	13104	153	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.

The worst 5 of 153 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:H:3:SER:N	3:H:223:HOH:O	2.07	0.86
1:E:3:SER:N	3:E:212:HOH:O	2.10	0.84
1:G:64:THR:HB	3:G:211:HOH:O	1.77	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:SER:N	3:C:207:HOH:O	2.17	0.78
1:G:145:LYS:HE2	3:G:224:HOH:O	1.88	0.74

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	199/204 (98%)	196 (98%)	3 (2%)	0	100	100
1	B	199/204 (98%)	192 (96%)	7 (4%)	0	100	100
1	C	199/204 (98%)	195 (98%)	4 (2%)	0	100	100
1	D	199/204 (98%)	195 (98%)	4 (2%)	0	100	100
1	E	199/204 (98%)	194 (98%)	5 (2%)	0	100	100
1	F	199/204 (98%)	195 (98%)	4 (2%)	0	100	100
1	G	199/204 (98%)	194 (98%)	5 (2%)	0	100	100
1	H	199/204 (98%)	193 (97%)	6 (3%)	0	100	100
All	All	1592/1632 (98%)	1554 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	181/184 (98%)	173 (96%)	8 (4%)	28	53
1	B	181/184 (98%)	171 (94%)	10 (6%)	21	43
1	C	181/184 (98%)	168 (93%)	13 (7%)	14	29
1	D	181/184 (98%)	168 (93%)	13 (7%)	14	29
1	E	181/184 (98%)	171 (94%)	10 (6%)	21	43
1	F	181/184 (98%)	171 (94%)	10 (6%)	21	43
1	G	181/184 (98%)	173 (96%)	8 (4%)	28	53
1	H	181/184 (98%)	168 (93%)	13 (7%)	14	29
All	All	1448/1472 (98%)	1363 (94%)	85 (6%)	19	39

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	33	LEU
1	G	191	ASN
1	F	107	SER
1	G	33	LEU
1	H	33	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	E	44	GLN
1	G	160	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	201/204 (98%)	0.33	4 (1%) 65 60	23, 33, 47, 49	0
1	B	201/204 (98%)	0.32	4 (1%) 65 60	22, 32, 46, 49	0
1	C	201/204 (98%)	0.39	12 (5%) 21 16	23, 33, 47, 49	0
1	D	201/204 (98%)	0.37	8 (3%) 38 31	23, 33, 46, 49	0
1	E	201/204 (98%)	0.16	5 (2%) 57 51	23, 33, 49, 53	0
1	F	201/204 (98%)	0.17	5 (2%) 57 51	23, 35, 48, 53	0
1	G	201/204 (98%)	0.30	9 (4%) 33 26	24, 35, 47, 49	0
1	H	201/204 (98%)	0.27	11 (5%) 25 19	23, 34, 46, 49	0
All	All	1608/1632 (98%)	0.29	58 (3%) 42 35	22, 34, 47, 53	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	127	SER	4.8
1	G	127	SER	4.4
1	G	191	ASN	4.3
1	C	124	PHE	4.2
1	C	190	TYR	4.2

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 monosaccharides 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
2	ZN	B	205	1/1	0.98	0.12	21,21,21,21	0
2	ZN	E	205	1/1	0.98	0.11	28,28,28,28	0
2	ZN	F	205	1/1	0.98	0.06	24,24,24,24	0
2	ZN	D	205	1/1	0.99	0.11	22,22,22,22	0
2	ZN	G	205	1/1	0.99	0.05	27,27,27,27	0
2	ZN	H	205	1/1	0.99	0.05	27,27,27,27	0
2	ZN	C	205	1/1	1.00	0.07	30,30,30,30	0
2	ZN	A	205	1/1	1.00	0.07	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.