



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:11 PM GMT

PDB ID : 4O2W
Title : Crystal structure of the third RCC1-like domain of HERC1
Authors : Dong, A.; Hu, J.; Li, Y.; Walker, J.R.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.M.; Tong, Y.; Structural Genomics Consortium (SGC)
Deposited on : 2013-12-17
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

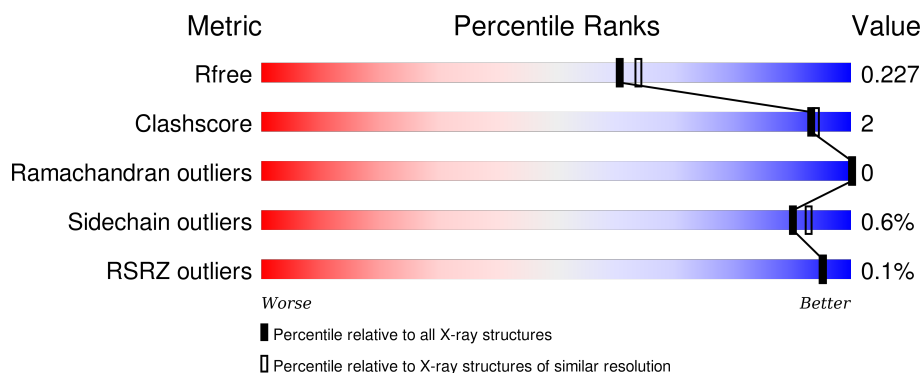
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	404	 86% 10%
1	B	404	 85% 5% 10%
1	C	404	 86% 10%
1	D	404	 85% 5% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNX	A	4408	-	-	-	X
4	UNX	A	4409	-	-	-	X
4	UNX	B	4402	-	-	-	X
4	UNX	B	4403	-	-	-	X
4	UNX	B	4405	-	-	-	X
4	UNX	C	4403	-	-	-	X
4	UNX	D	4405	-	-	-	X
4	UNX	D	4409	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11463 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 E3 ubiquitin-protein ligase HERC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	9	0
			2725	1689	493	529	14			
1	B	365	Total	C	N	O	S	0	6	0
			2692	1669	489	519	15			
1	C	365	Total	C	N	O	S	0	3	0
			2663	1655	480	514	14			
1	D	364	Total	C	N	O	S	0	3	0
			2672	1657	481	520	14			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3957	MET	-	EXPRESSION TAG	UNP Q15751
A	3958	HIS	-	EXPRESSION TAG	UNP Q15751
A	3959	HIS	-	EXPRESSION TAG	UNP Q15751
A	3960	HIS	-	EXPRESSION TAG	UNP Q15751
A	3961	HIS	-	EXPRESSION TAG	UNP Q15751
A	3962	HIS	-	EXPRESSION TAG	UNP Q15751
A	3963	HIS	-	EXPRESSION TAG	UNP Q15751
A	3964	SER	-	EXPRESSION TAG	UNP Q15751
A	3965	SER	-	EXPRESSION TAG	UNP Q15751
A	3966	GLY	-	EXPRESSION TAG	UNP Q15751
A	3967	ARG	-	EXPRESSION TAG	UNP Q15751
A	3968	GLU	-	EXPRESSION TAG	UNP Q15751
A	3969	ASN	-	EXPRESSION TAG	UNP Q15751
A	3970	LEU	-	EXPRESSION TAG	UNP Q15751
A	3971	TYR	-	EXPRESSION TAG	UNP Q15751
A	3972	PHE	-	EXPRESSION TAG	UNP Q15751
A	3973	GLN	-	EXPRESSION TAG	UNP Q15751
A	3974	GLY	-	EXPRESSION TAG	UNP Q15751
B	3957	MET	-	EXPRESSION TAG	UNP Q15751
B	3958	HIS	-	EXPRESSION TAG	UNP Q15751
B	3959	HIS	-	EXPRESSION TAG	UNP Q15751

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3960	HIS	-	EXPRESSION TAG	UNP Q15751
B	3961	HIS	-	EXPRESSION TAG	UNP Q15751
B	3962	HIS	-	EXPRESSION TAG	UNP Q15751
B	3963	HIS	-	EXPRESSION TAG	UNP Q15751
B	3964	SER	-	EXPRESSION TAG	UNP Q15751
B	3965	SER	-	EXPRESSION TAG	UNP Q15751
B	3966	GLY	-	EXPRESSION TAG	UNP Q15751
B	3967	ARG	-	EXPRESSION TAG	UNP Q15751
B	3968	GLU	-	EXPRESSION TAG	UNP Q15751
B	3969	ASN	-	EXPRESSION TAG	UNP Q15751
B	3970	LEU	-	EXPRESSION TAG	UNP Q15751
B	3971	TYR	-	EXPRESSION TAG	UNP Q15751
B	3972	PHE	-	EXPRESSION TAG	UNP Q15751
B	3973	GLN	-	EXPRESSION TAG	UNP Q15751
B	3974	GLY	-	EXPRESSION TAG	UNP Q15751
C	3957	MET	-	EXPRESSION TAG	UNP Q15751
C	3958	HIS	-	EXPRESSION TAG	UNP Q15751
C	3959	HIS	-	EXPRESSION TAG	UNP Q15751
C	3960	HIS	-	EXPRESSION TAG	UNP Q15751
C	3961	HIS	-	EXPRESSION TAG	UNP Q15751
C	3962	HIS	-	EXPRESSION TAG	UNP Q15751
C	3963	HIS	-	EXPRESSION TAG	UNP Q15751
C	3964	SER	-	EXPRESSION TAG	UNP Q15751
C	3965	SER	-	EXPRESSION TAG	UNP Q15751
C	3966	GLY	-	EXPRESSION TAG	UNP Q15751
C	3967	ARG	-	EXPRESSION TAG	UNP Q15751
C	3968	GLU	-	EXPRESSION TAG	UNP Q15751
C	3969	ASN	-	EXPRESSION TAG	UNP Q15751
C	3970	LEU	-	EXPRESSION TAG	UNP Q15751
C	3971	TYR	-	EXPRESSION TAG	UNP Q15751
C	3972	PHE	-	EXPRESSION TAG	UNP Q15751
C	3973	GLN	-	EXPRESSION TAG	UNP Q15751
C	3974	GLY	-	EXPRESSION TAG	UNP Q15751
D	3957	MET	-	EXPRESSION TAG	UNP Q15751
D	3958	HIS	-	EXPRESSION TAG	UNP Q15751
D	3959	HIS	-	EXPRESSION TAG	UNP Q15751
D	3960	HIS	-	EXPRESSION TAG	UNP Q15751
D	3961	HIS	-	EXPRESSION TAG	UNP Q15751
D	3962	HIS	-	EXPRESSION TAG	UNP Q15751
D	3963	HIS	-	EXPRESSION TAG	UNP Q15751
D	3964	SER	-	EXPRESSION TAG	UNP Q15751
D	3965	SER	-	EXPRESSION TAG	UNP Q15751

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Chain	Residue	Modelled	Actual	Comment	Reference
D	3966	GLY	-	EXPRESSION TAG	UNP Q15751
D	3967	ARG	-	EXPRESSION TAG	UNP Q15751
D	3968	GLU	-	EXPRESSION TAG	UNP Q15751
D	3969	ASN	-	EXPRESSION TAG	UNP Q15751
D	3970	LEU	-	EXPRESSION TAG	UNP Q15751
D	3971	TYR	-	EXPRESSION TAG	UNP Q15751
D	3972	PHE	-	EXPRESSION TAG	UNP Q15751
D	3973	GLN	-	EXPRESSION TAG	UNP Q15751
D	3974	GLY	-	EXPRESSION TAG	UNP Q15751

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3 3	0	0
3	D	2	Total Cl 2 2	0	0

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	9	Total X 9 9	0	0
4	A	5	Total X 5 5	0	0
4	D	8	Total X 8 8	0	0
4	C	3	Total X 3 3	0	0

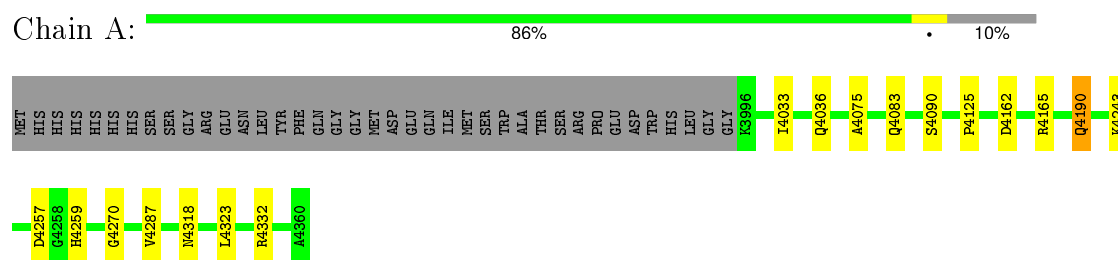
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	194	Total 196	O 196	0	2
5	B	173	Total 174	O 174	0	1
5	C	130	Total 130	O 130	0	0
5	D	176	Total 178	O 178	0	2

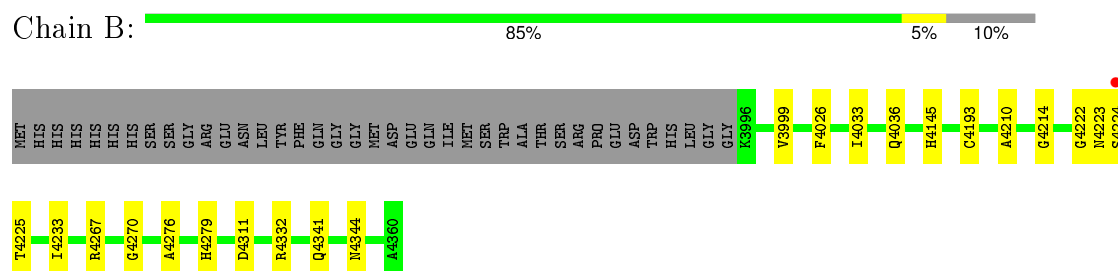
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

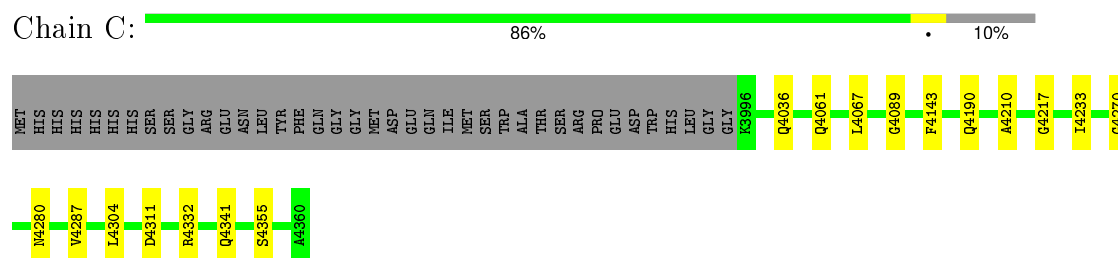
- Molecule 1: E3 ubiquitin-protein ligase HERC1



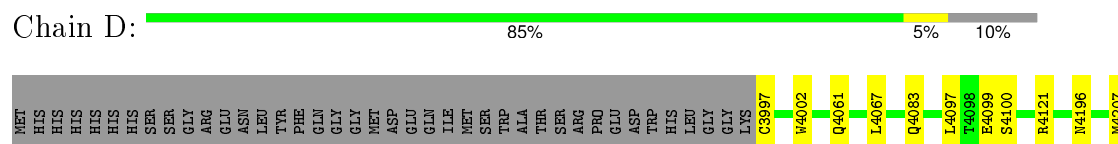
- Molecule 1: E3 ubiquitin-protein ligase HERC1



- Molecule 1: E3 ubiquitin-protein ligase HERC1



- Molecule 1: E3 ubiquitin-protein ligase HERC1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.38Å 70.90Å 105.55Å 70.93° 81.26° 90.84°	Depositor
Resolution (Å)	50.00 – 2.00 42.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.00) 88.7 (42.81-2.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049, COOT 0.7.1	Depositor
R, R_{free}	0.181 , 0.221 0.189 , 0.227	Depositor DCC
R_{free} test set	980 reflections (1.02%)	DCC
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 18.4	EDS
Estimated twinning fraction	0.096 for -h,k,k-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 97126 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11463	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: UNX, MG, CL

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	0.48	0/2789	0.64	0/3774
1	B	0.50	0/2758	0.68	0/3732
1	C	0.44	0/2717	0.64	0/3683
1	D	0.49	0/2729	0.67	1/3696 (0.0%)
All	All	0.48	0/10993	0.65	1/14885 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4121	ARG	NE-CZ-NH2	-5.59	117.51	120.30

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	2725	0	2642	10	0
1	B	2692	0	2622	12	0
1	C	2663	0	2560	8	0
1	D	2672	0	2586	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
3	A	3	0	0	0	0
3	D	2	0	0	0	0
4	A	5	0	0	0	0
4	B	9	0	0	0	0
4	C	3	0	0	0	0
4	D	8	0	0	0	0
5	A	196	0	0	2	0
5	B	174	0	0	2	0
5	C	130	0	0	1	0
5	D	178	0	0	1	0
All	All	11463	0	10410	41	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.

The worst 5 of 41 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:4083:GLN:HG3	5:A:4641:HOH:O	1.88	0.74
1:C:4311:ASP:OD1	1:C:4341:GLN:NE2	2.22	0.73
1:B:4223:ASN:OD1	1:B:4225:THR:HG22	1.98	0.64
1:D:4083:GLN:HE21	1:D:4097:LEU:HD23	1.64	0.60
1:A:4287[A]:VAL:HG22	5:A:4529:HOH:O	2.05	0.57

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	372/404 (92%)	362 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	369/404 (91%)	361 (98%)	8 (2%)	0	100	100
1	C	366/404 (91%)	356 (97%)	10 (3%)	0	100	100
1	D	365/404 (90%)	353 (97%)	12 (3%)	0	100	100
All	All	1472/1616 (91%)	1432 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	283/312 (91%)	282 (100%)	1 (0%)	93	95
1	B	278/312 (89%)	276 (99%)	2 (1%)	88	91
1	C	269/312 (86%)	267 (99%)	2 (1%)	88	91
1	D	275/312 (88%)	274 (100%)	1 (0%)	93	95
All	All	1105/1248 (88%)	1099 (100%)	6 (0%)	90	94

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4267	ARG
1	D	3997	CYS
1	C	4036	GLN
1	B	4036	GLN
1	C	4190	GLN

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

Mol	Chain	Res	Type
1	C	4043	GLN
1	D	4083	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 25 are unknown and 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	365/404 (90%)	-0.72	0 100 100	9, 16, 27, 41	0
1	B	365/404 (90%)	-0.73	1 (0%) 94 94	10, 16, 29, 40	0
1	C	365/404 (90%)	-0.63	0 100 100	12, 22, 38, 52	0
1	D	364/404 (90%)	-0.71	1 (0%) 94 94	10, 17, 30, 36	0
All	All	1459/1616 (90%)	-0.70	2 (0%) 95 95	9, 18, 32, 52	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4224	SER	3.0
1	D	4360	ALA	2.2

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	UNX	B	4403	1/1	0.84	0.38	22.94	30,30,30,30	0
4	UNX	B	4402	1/1	0.55	0.24	19.93	30,30,30,30	0
4	UNX	A	4408	1/1	0.98	0.30	12.50	30,30,30,30	0
4	UNX	D	4405	1/1	0.97	0.16	11.09	30,30,30,30	0
4	UNX	C	4403	1/1	0.87	0.24	11.08	30,30,30,30	0
4	UNX	D	4409	1/1	0.97	0.30	6.31	30,30,30,30	0
4	UNX	A	4409	1/1	0.85	0.14	6.19	30,30,30,30	0
4	UNX	B	4405	1/1	0.89	0.20	6.15	30,30,30,30	0
3	CL	A	4403	1/1	0.99	0.11	1.70	37,37,37,37	0
3	CL	D	4402	1/1	0.99	0.08	-0.46	35,35,35,35	0
3	CL	A	4404	1/1	0.99	0.06	-0.99	15,15,15,15	0
3	CL	D	4403	1/1	1.00	0.03	-1.64	28,28,28,28	0
3	CL	A	4402	1/1	0.98	0.03	-1.82	34,34,34,34	0
2	MG	D	4401	1/1	0.99	0.04	-	27,27,27,27	0
4	UNX	C	4401	1/1	0.90	0.16	-	30,30,30,30	0
4	UNX	D	4410	1/1	0.61	0.34	-	30,30,30,30	0
4	UNX	B	4409	1/1	0.89	0.17	-	30,30,30,30	0
4	UNX	D	4408	1/1	0.75	0.34	-	30,30,30,30	0
4	UNX	B	4408	1/1	0.97	0.16	-	30,30,30,30	0
4	UNX	D	4411	1/1	0.93	0.17	-	30,30,30,30	0
4	UNX	A	4407	1/1	0.71	0.28	-	30,30,30,30	0
2	MG	A	4401	1/1	0.96	0.03	-	30,30,30,30	0
4	UNX	A	4405	1/1	0.94	0.16	-	30,30,30,30	0
4	UNX	B	4410	1/1	0.92	0.37	-	30,30,30,30	0
4	UNX	D	4404	1/1	0.91	0.14	-	30,30,30,30	0
4	UNX	B	4407	1/1	0.94	0.07	-	30,30,30,30	0
4	UNX	D	4407	1/1	0.92	0.37	-	30,30,30,30	0
4	UNX	A	4406	1/1	0.94	0.39	-	30,30,30,30	0
2	MG	B	4401	1/1	0.96	0.04	-	30,30,30,30	0
4	UNX	B	4406	1/1	0.97	0.25	-	30,30,30,30	0
4	UNX	D	4406	1/1	0.91	0.26	-	30,30,30,30	0
4	UNX	C	4402	1/1	0.81	0.21	-	30,30,30,30	0
4	UNX	B	4404	1/1	0.91	0.26	-	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.