



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 04:20 PM EDT

PDB ID : 4IXT
Title : Structure of a 37-fold mutant of halohydrin dehalogenase (HheC) bound to ethyl (R)-4-cyano-3-hydroxybutyrate
Authors : Floor, R.J.; Schallmeyer, M.; Hauer, B.; Breuer, M.; Jekel, P.A.; Wijma, H.J.; Dijkstra, B.W.; Janssen, D.B.
Deposited on : 2013-01-28
Resolution : 2.49 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

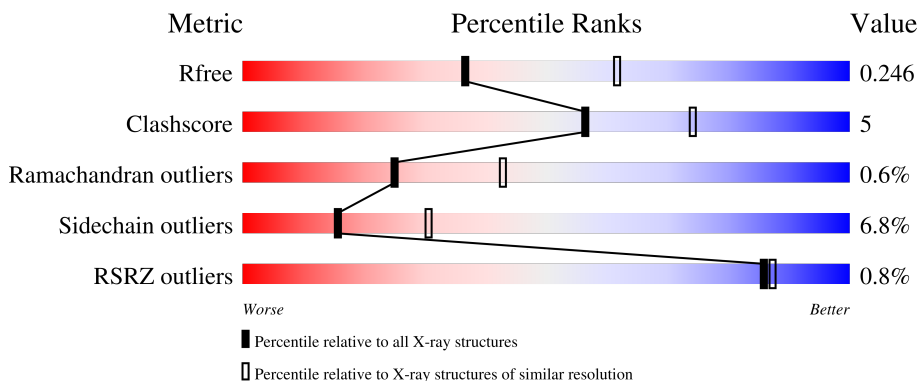
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	254	 84% 13% ..
1	B	254	 81% 13% ..

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 3877 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 Halohydrin dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	249	1926	1232	323	365	6	0	0	0
1	B	245	1885	1205	315	359	6	0	0	0

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	GLN	engineered mutation	UNP Q93D82
A	38	GLN	LYS	engineered mutation	UNP Q93D82
A	52	ILE	LYS	engineered mutation	UNP Q93D82
A	60	VAL	ALA	engineered mutation	UNP Q93D82
A	70	LEU	TYR	engineered mutation	UNP Q93D82
A	72	HIS	GLN	engineered mutation	UNP Q93D82
A	75	ILE	VAL	engineered mutation	UNP Q93D82
A	82	ALA	PHE	engineered mutation	UNP Q93D82
A	83	PRO	ALA	engineered mutation	UNP Q93D82
A	84	VAL	PRO	engineered mutation	UNP Q93D82
A	86	TRP	PHE	engineered mutation	UNP Q93D82
A	87	ARG	GLN	engineered mutation	UNP Q93D82
A	99	ASP	GLY	engineered mutation	UNP Q93D82
A	100	MET	ALA	engineered mutation	UNP Q93D82
A	107	LYS	ARG	engineered mutation	UNP Q93D82
A	112	ALA	VAL	engineered mutation	UNP Q93D82
A	121	ARG	LYS	engineered mutation	UNP Q93D82
A	134	ALA	THR	engineered mutation	UNP Q93D82
A	135	SER	PRO	engineered mutation	UNP Q93D82
A	146	ALA	THR	engineered mutation	UNP Q93D82
A	153	SER	CYS	engineered mutation	UNP Q93D82
A	154	ALA	THR	engineered mutation	UNP Q93D82
A	166	HIS	TYR	engineered mutation	UNP Q93D82
A	174	ALA	GLY	engineered mutation	UNP Q93D82
A	177	GLY	TYR	engineered mutation	UNP Q93D82

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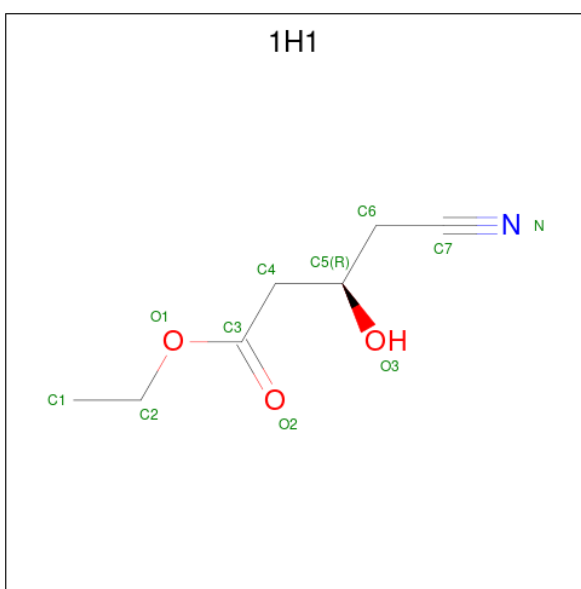
Chain	Residue	Modelled	Actual	Comment	Reference
A	178	VAL	LEU	engineered mutation	UNP Q93D82
A	179	ASP	HIS	engineered mutation	UNP Q93D82
A	181	GLY	GLU	engineered mutation	UNP Q93D82
A	186	TYR	PHE	engineered mutation	UNP Q93D82
A	189	SER	THR	engineered mutation	UNP Q93D82
A	195	SER	ASN	engineered mutation	UNP Q93D82
A	201	TRP	HIS	engineered mutation	UNP Q93D82
A	203	ARG	LYS	engineered mutation	UNP Q93D82
A	205	TYR	VAL	engineered mutation	UNP Q93D82
A	222	THR	ALA	engineered mutation	UNP Q93D82
A	245	VAL	MET	engineered mutation	UNP Q93D82
A	246	VAL	ILE	engineered mutation	UNP Q93D82
B	37	HIS	GLN	engineered mutation	UNP Q93D82
B	38	GLN	LYS	engineered mutation	UNP Q93D82
B	52	ILE	LYS	engineered mutation	UNP Q93D82
B	60	VAL	ALA	engineered mutation	UNP Q93D82
B	70	LEU	TYR	engineered mutation	UNP Q93D82
B	72	HIS	GLN	engineered mutation	UNP Q93D82
B	75	ILE	VAL	engineered mutation	UNP Q93D82
B	82	ALA	PHE	engineered mutation	UNP Q93D82
B	83	PRO	ALA	engineered mutation	UNP Q93D82
B	84	VAL	PRO	engineered mutation	UNP Q93D82
B	86	TRP	PHE	engineered mutation	UNP Q93D82
B	87	ARG	GLN	engineered mutation	UNP Q93D82
B	99	ASP	GLY	engineered mutation	UNP Q93D82
B	100	MET	ALA	engineered mutation	UNP Q93D82
B	107	LYS	ARG	engineered mutation	UNP Q93D82
B	112	ALA	VAL	engineered mutation	UNP Q93D82
B	121	ARG	LYS	engineered mutation	UNP Q93D82
B	134	ALA	THR	engineered mutation	UNP Q93D82
B	135	SER	PRO	engineered mutation	UNP Q93D82
B	146	ALA	THR	engineered mutation	UNP Q93D82
B	153	SER	CYS	engineered mutation	UNP Q93D82
B	154	ALA	THR	engineered mutation	UNP Q93D82
B	166	HIS	TYR	engineered mutation	UNP Q93D82
B	174	ALA	GLY	engineered mutation	UNP Q93D82
B	177	GLY	TYR	engineered mutation	UNP Q93D82
B	178	VAL	LEU	engineered mutation	UNP Q93D82
B	179	ASP	HIS	engineered mutation	UNP Q93D82
B	181	GLY	GLU	engineered mutation	UNP Q93D82
B	186	TYR	PHE	engineered mutation	UNP Q93D82
B	189	SER	THR	engineered mutation	UNP Q93D82

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Chain	Residue	Modelled	Actual	Comment	Reference
B	195	SER	ASN	engineered mutation	UNP Q93D82
B	201	TRP	HIS	engineered mutation	UNP Q93D82
B	203	ARG	LYS	engineered mutation	UNP Q93D82
B	205	TYR	VAL	engineered mutation	UNP Q93D82
B	222	THR	ALA	engineered mutation	UNP Q93D82
B	245	VAL	MET	engineered mutation	UNP Q93D82
B	246	VAL	ILE	engineered mutation	UNP Q93D82

- Molecule 2 is ethyl (3R)-4-cyano-3-hydroxybutanoate (three-letter code: 1H1) (formula: $C_7H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	7	1	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		

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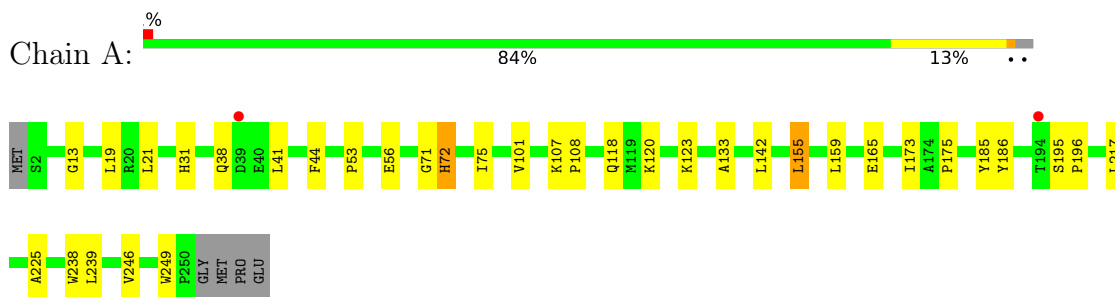
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	28	Total	O	0	0
			28	28		

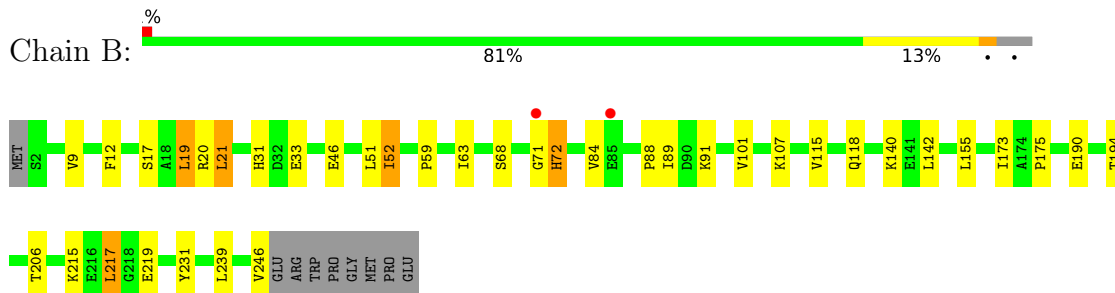
3 Residue-property plots [i](#)

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: Halohydrin dehalogenase



- Molecule 1: Halohydrin dehalogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.68Å 104.68Å 121.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.34 – 2.49 46.82 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.34-2.49) 99.9 (46.82-2.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.88 (at 2.48Å)	Xtrriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.199 , 0.249 0.195 , 0.246	Depositor DCC
R_{free} test set	1232 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3877	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: CL, 1H1

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	0.49	0/1979	0.57	0/2697
1	B	0.48	0/1935	0.56	0/2636
All	All	0.49	0/3914	0.56	0/5333

There are no bond length outliers.

There are no bond angle outliers.

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	1926	0	1870	20	0
1	B	1885	0	1834	20	0
2	A	11	0	11	3	0
3	B	1	0	0	0	0
4	A	26	0	0	0	0
4	B	28	0	0	0	0
All	All	3877	0	3715	38	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 5.

All (38) 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:142:LEU:HD21	2:A:301:1H1:C1	2.07	0.85
1:A:142:LEU:HD21	2:A:301:1H1:H4	1.60	0.84
1:B:84:VAL:HG21	1:B:142:LEU:HD11	1.71	0.72
1:B:71:GLY:O	1:B:72:HIS:HB2	1.90	0.71
1:B:71:GLY:O	1:B:72:HIS:CB	2.45	0.64
1:B:84:VAL:CG2	1:B:142:LEU:HD11	2.30	0.61
1:B:52:ILE:HG13	1:B:52:ILE:O	1.99	0.60
1:A:133:ALA:HA	1:A:238:TRP:CZ3	2.38	0.59
1:B:17:SER:O	1:B:21:LEU:HD22	2.04	0.57
1:A:173:ILE:O	1:A:175:PRO:HD3	2.05	0.57
1:B:88:PRO:HG2	1:B:91:LYS:HG2	1.88	0.55
1:A:71:GLY:O	1:A:72:HIS:HB3	2.05	0.55
1:B:52:ILE:O	1:B:52:ILE:CG1	2.57	0.53
1:A:159:LEU:HD21	1:B:89:ILE:HD13	1.93	0.51
1:A:41:LEU:C	1:A:41:LEU:HD23	2.31	0.50
1:A:142:LEU:HD21	2:A:301:1H1:H3	1.93	0.49
1:B:173:ILE:O	1:B:175:PRO:HD3	2.13	0.48
1:B:215:LYS:O	1:B:219:GLU:HG2	2.14	0.48
1:A:120:LYS:O	1:A:123:LYS:HD2	2.15	0.47
1:A:44:PHE:HD2	1:A:53:PRO:HG3	1.80	0.47
1:B:59:PRO:O	1:B:63:ILE:HG12	2.15	0.46
1:B:190:GLU:OE2	1:B:194:THR:HG21	2.16	0.46
1:A:107:LYS:HB3	1:A:108:PRO:HD3	1.98	0.46
1:A:101:VAL:HG11	1:B:101:VAL:HG11	1.98	0.46
1:A:185:TYR:HA	1:A:186:TYR:HA	1.76	0.46
1:A:71:GLY:O	1:A:72:HIS:CB	2.65	0.45
1:B:9:VAL:O	1:B:9:VAL:HG22	2.17	0.44
1:B:246:VAL:O	1:B:246:VAL:HG23	2.17	0.44
1:A:13:GLY:HA3	1:A:217:LEU:HD21	1.99	0.44
1:A:75:ILE:HD13	1:A:225:ALA:HB1	1.98	0.44
1:B:142:LEU:HD12	1:B:142:LEU:HA	1.88	0.44
1:B:217:LEU:C	1:B:217:LEU:CD1	2.87	0.43
1:A:195:SER:HA	1:A:196:PRO:HD3	1.78	0.43
1:B:19:LEU:HD13	1:B:51:LEU:HD11	2.01	0.42
1:B:71:GLY:O	1:B:72:HIS:CG	2.72	0.42
1:A:107:LYS:HB3	1:A:108:PRO:CD	2.50	0.42
1:A:56:GLU:OE2	1:A:56:GLU:N	2.43	0.42
1:A:155:LEU:HD22	1:A:159:LEU:HG	2.02	0.42

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	247/254 (97%)	233 (94%)	12 (5%)	2 (1%)	19	35
1	B	243/254 (96%)	231 (95%)	11 (4%)	1 (0%)	34	54
All	All	490/508 (96%)	464 (95%)	23 (5%)	3 (1%)	25	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	HIS
1	A	72	HIS
1	A	249	TRP

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	202/206 (98%)	193 (96%)	9 (4%)	27	51
1	B	198/206 (96%)	180 (91%)	18 (9%)	9	18
All	All	400/412 (97%)	373 (93%)	27 (7%)	16	30

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	21	LEU
1	A	31	HIS

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Mol	Chain	Res	Type
1	A	38	GLN
1	A	118	GLN
1	A	155	LEU
1	A	165	GLU
1	A	239	LEU
1	A	246	VAL
1	B	12	PHE
1	B	19	LEU
1	B	20	ARG
1	B	21	LEU
1	B	31	HIS
1	B	33	GLU
1	B	46	GLU
1	B	52	ILE
1	B	68	SER
1	B	107	LYS
1	B	115	VAL
1	B	118	GLN
1	B	140	LYS
1	B	155	LEU
1	B	206	THR
1	B	217	LEU
1	B	231	TYR
1	B	239	LEU

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

Mol	Chain	Res	Type
1	A	72	HIS
1	B	176	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	1H1	A	301	-	10,10,10	1.47	1 (10%)	10,11,11	1.99	1 (10%)

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	1H1	A	301	-	-	2/9/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	1H1	O1-C3	4.35	1.46	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	1H1	O1-C3-C4	5.49	120.87	111.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	1H1	C4-C3-O1-C2

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Mol	Chain	Res	Type	Atoms
2	A	301	1H1	O2-C3-O1-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	1H1	3	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 [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	249/254 (98%)	-0.42	2 (0%) 86 87	13, 26, 52, 70	0
1	B	245/254 (96%)	-0.60	2 (0%) 86 87	12, 24, 49, 62	0
All	All	494/508 (97%)	-0.51	4 (0%) 86 87	12, 25, 51, 70	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	GLY	2.9
1	A	39	ASP	2.8
1	A	194	THR	2.1
1	B	85	GLU	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 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	1H1	A	301	11/11	0.94	0.12	19,32,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	B	301	1/1	0.98	0.13	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.