



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:30 am GMT

PDB ID : 1M13
Title : Crystal Structure of the Human Pregane X Receptor Ligand Binding Domain
in Complex with Hyperforin, a Constituent of St. John's Wort
Authors : Watkins, R.E.; Maglich, J.M.; Moore, L.B.; Wisely, G.B.; Noble, S.M.; Davis-
Searles, P.R.; Lambert, M.H.; Kliewer, S.A.; Redinbo, M.R.
Deposited on : 2002-06-17
Resolution : 2.15 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

<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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

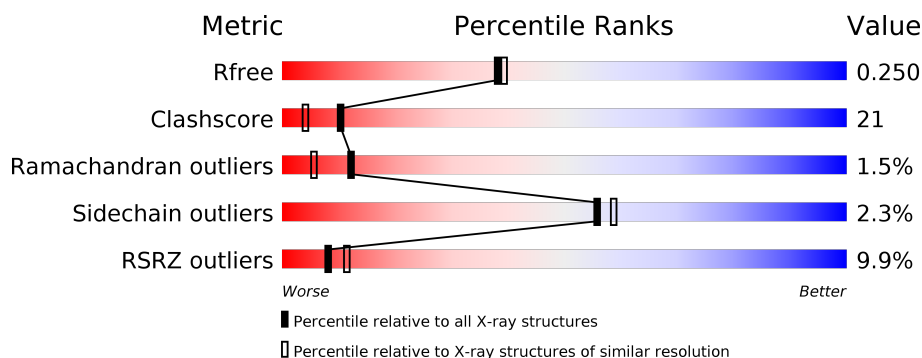
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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	316	<div> <div>9%</div> <div>61%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>

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
2	HYF	A	435	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2450 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.

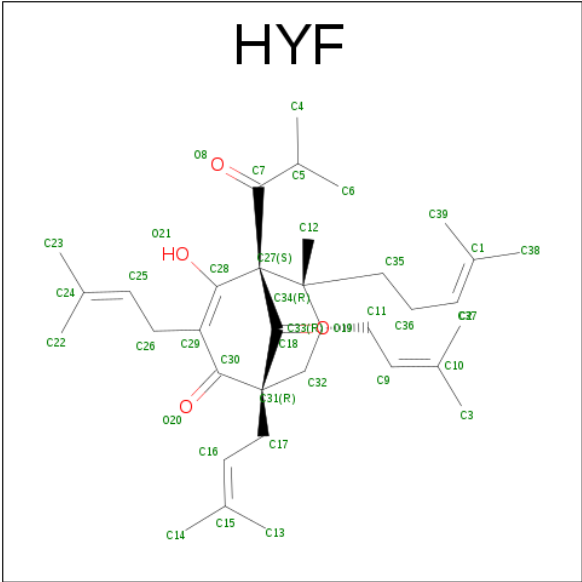
- Molecule 1 is a protein called Orphan Nuclear Receptor PXR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	2146	1380	365	383	18	0	1	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MET	-	EXPRESSION TAG	UNP O75469
A	120	LYS	-	EXPRESSION TAG	UNP O75469
A	121	LYS	-	EXPRESSION TAG	UNP O75469
A	122	GLY	-	EXPRESSION TAG	UNP O75469
A	123	HIS	-	EXPRESSION TAG	UNP O75469
A	124	HIS	-	EXPRESSION TAG	UNP O75469
A	125	HIS	-	EXPRESSION TAG	UNP O75469
A	126	HIS	-	EXPRESSION TAG	UNP O75469
A	127	HIS	-	EXPRESSION TAG	UNP O75469
A	128	HIS	-	EXPRESSION TAG	UNP O75469
A	129	GLY	-	EXPRESSION TAG	UNP O75469

- Molecule 2 is 4-HYDROXY-5-ISOBUTYRYL-6-METHYL-1,3,7-TRIS-(3-METHYL-BUT-2-ENYL)-6-(4-METHYL-PENT-3-ENYL)-BICYCLO[3.3.1]NON-3-ENE-2,9-DIONE (three-letter code: HYF) (formula: C₃₅H₅₂O₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	O	0
			39	35	4	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	265	Total	O	0	0
			265	265		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.37Å 91.37Å 85.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.15 19.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.87-2.15) 99.6 (19.87-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.51 (at 2.09Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.246 0.213 , 0.250	Depositor DCC
R_{free} test set	998 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2450	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: HYF

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	0.34	0/2193	0.54	0/2963

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 [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	2146	0	2085	80	0
2	A	39	0	52	28	0
3	A	265	0	0	13	0
All	All	2450	0	2137	90	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 21.

All (90) 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)
2:A:435:HYF:C33	2:A:435:HYF:C34	1.80	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:435:HYF:C27	2:A:435:HYF:C34	1.80	1.56
1:A:215:LEU:HD22	1:A:304:LEU:HD22	1.30	1.14
1:A:284[A]:CYS:SG	2:A:435:HYF:H043	1.93	1.08
1:A:243:MET:HB3	2:A:435:HYF:H121	1.51	0.91
1:A:215:LEU:CD2	1:A:304:LEU:HD22	2.10	0.79
2:A:435:HYF:C33	2:A:435:HYF:C12	2.60	0.78
1:A:214:GLN:HE21	1:A:216:ARG:HH11	1.30	0.78
2:A:435:HYF:C18	2:A:435:HYF:C34	2.62	0.77
2:A:435:HYF:C35	2:A:435:HYF:C33	2.71	0.67
1:A:154:LEU:HD13	3:A:488:HOH:O	1.94	0.67
2:A:435:HYF:C28	2:A:435:HYF:C34	2.74	0.65
1:A:145:GLU:O	1:A:149:MET:HG3	1.99	0.62
1:A:210:LYS:HB3	1:A:309:GLU:HB2	1.82	0.61
1:A:214:GLN:NE2	1:A:216:ARG:HH11	2.00	0.60
1:A:289:ASN:HD22	1:A:327:HIS:HD1	1.49	0.60
1:A:234:LYS:O	1:A:236:ILE:N	2.35	0.60
1:A:304:LEU:HG	3:A:587:HOH:O	2.02	0.59
1:A:254:ILE:HD12	1:A:283:LEU:HB3	1.85	0.58
1:A:213:LEU:HD21	1:A:215:LEU:HD21	1.85	0.57
2:A:435:HYF:C27	2:A:435:HYF:C12	2.77	0.57
1:A:283:LEU:CD1	1:A:344:GLN:HB3	2.34	0.57
1:A:288:PHE:CD1	2:A:435:HYF:H382	2.40	0.57
2:A:435:HYF:C32	2:A:435:HYF:C34	2.78	0.56
1:A:152:ARG:HD2	3:A:508:HOH:O	2.06	0.55
1:A:144:THR:OG1	1:A:147:GLN:HG3	2.06	0.55
1:A:312:ALA:HB3	3:A:653:HOH:O	2.07	0.55
1:A:240:LEU:CD2	2:A:435:HYF:H142	2.37	0.54
1:A:213:LEU:HD21	1:A:215:LEU:CD2	2.37	0.54
1:A:381:ARG:NH2	3:A:530:HOH:O	2.39	0.54
1:A:206:LEU:HD12	1:A:206:LEU:H	1.74	0.53
2:A:435:HYF:H331	2:A:435:HYF:C12	2.37	0.53
1:A:323:MET:HG2	2:A:435:HYF:C24	2.39	0.53
1:A:206:LEU:HD12	1:A:206:LEU:N	2.24	0.53
1:A:298:THR:HG22	1:A:307:CYS:SG	2.50	0.52
1:A:361:VAL:HG23	3:A:487:HOH:O	2.09	0.51
1:A:260:VAL:HG13	3:A:516:HOH:O	2.10	0.51
1:A:273:ILE:O	1:A:277:LYS:HG3	2.10	0.51
2:A:435:HYF:O21	2:A:435:HYF:H051	2.10	0.51
1:A:296:THR:O	1:A:298:THR:HG23	2.11	0.50
1:A:284[A]:CYS:SG	2:A:435:HYF:H062	2.51	0.50
1:A:243:MET:HB3	2:A:435:HYF:C12	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:O	1:A:235:GLU:C	2.50	0.50
1:A:323:MET:HG2	2:A:435:HYF:C25	2.42	0.49
1:A:251:PHE:CD2	1:A:284[B]:CYS:SG	3.06	0.49
1:A:152:ARG:HG2	3:A:658:HOH:O	2.12	0.48
1:A:207:CYS:C	1:A:209:LEU:H	2.17	0.48
1:A:324:LEU:HD12	1:A:328:TYR:HE1	1.77	0.48
1:A:284[A]:CYS:SG	2:A:435:HYF:C4	2.85	0.48
1:A:206:LEU:O	1:A:209:LEU:HB2	2.13	0.48
1:A:263:TYR:HE1	3:A:488:HOH:O	1.96	0.48
1:A:411:LEU:HD23	1:A:411:LEU:C	2.35	0.47
1:A:282:GLU:HG2	1:A:400:LEU:HG	1.96	0.47
1:A:319:LEU:O	1:A:325:LYS:HB2	2.14	0.47
1:A:285:GLN:NE2	1:A:327:HIS:NE2	2.62	0.47
1:A:352:ASP:O	1:A:401:ARG:NH2	2.48	0.47
1:A:203:ARG:C	1:A:205:ASP:H	2.19	0.47
1:A:257:PHE:O	1:A:260:VAL:HG22	2.15	0.47
1:A:243:MET:HG3	2:A:435:HYF:C2	2.45	0.47
1:A:384:PRO:HB3	3:A:463:HOH:O	2.15	0.46
1:A:243:MET:HG3	2:A:435:HYF:H021	1.97	0.46
1:A:213:LEU:C	1:A:213:LEU:HD23	2.35	0.46
1:A:349:PHE:O	1:A:366:GLN:HB2	2.15	0.46
1:A:206:LEU:CD1	1:A:206:LEU:H	2.28	0.46
1:A:247:SER:HA	2:A:435:HYF:H041	1.98	0.46
1:A:152:ARG:HD2	3:A:454:HOH:O	2.15	0.46
1:A:414:ILE:HD12	2:A:435:HYF:H143	1.97	0.46
1:A:203:ARG:O	1:A:206:LEU:HD13	2.16	0.45
1:A:240:LEU:HB2	1:A:241:PRO:HD3	1.98	0.45
1:A:150:MET:HE1	3:A:524:HOH:O	2.17	0.44
1:A:240:LEU:HD21	2:A:435:HYF:H142	1.98	0.44
1:A:315:PHE:O	1:A:319:LEU:HG	2.17	0.44
1:A:199:TRP:CB	1:A:417:ILE:HD11	2.47	0.44
1:A:259:LYS:O	1:A:265:ARG:HG3	2.18	0.43
1:A:216:ARG:O	1:A:303:ARG:HD2	2.18	0.43
1:A:352:ASP:OD2	1:A:401:ARG:NH2	2.52	0.43
1:A:209:LEU:HD22	2:A:435:HYF:C9	2.48	0.43
1:A:284[A]:CYS:HB3	2:A:435:HYF:H062	2.00	0.43
1:A:217:GLY:C	1:A:219:ASP:H	2.20	0.43
1:A:233:GLY:O	1:A:234:LYS:C	2.57	0.43
1:A:425:MET:O	1:A:429:PHE:HD1	2.01	0.43
1:A:211:VAL:HA	1:A:307:CYS:O	2.19	0.42
1:A:414:ILE:CD1	2:A:435:HYF:H143	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:SER:HA	2:A:435:HYF:C4	2.50	0.41
1:A:209:LEU:O	1:A:210:LYS:HG2	2.21	0.41
1:A:399:GLU:HA	1:A:399:GLU:OE1	2.21	0.41
1:A:215:LEU:HD22	1:A:304:LEU:CD2	2.23	0.40
1:A:149:MET:HB2	3:A:564:HOH:O	2.22	0.40
1:A:211:VAL:O	1:A:211:VAL:HG23	2.20	0.40
1:A:403:ILE:HG23	1:A:407:HIS:CD2	2.57	0.40

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	270/316 (85%)	252 (93%)	14 (5%)	4 (2%)	12 5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	LYS
1	A	235	GLU
1	A	208	SER
1	A	312	ALA

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	223/279 (80%)	218 (98%)	5 (2%)	57 60

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LEU
1	A	154	LEU
1	A	159	MET
1	A	324	LEU
1	A	360	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	214	GLN
1	A	272	GLN
1	A	285	GLN
1	A	364	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	HYF	A	435	-	37,40,40	3.41	15 (40%)	46,61,61	2.22	9 (19%)

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	HYF	A	435	-	-	2/33/85/85	0/0/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	435	HYF	C12-C34	2.05	1.58	1.54
2	A	435	HYF	C35-C34	2.11	1.59	1.55
2	A	435	HYF	O21-C28	2.20	1.40	1.32
2	A	435	HYF	C26-C29	2.69	1.56	1.51
2	A	435	HYF	C17-C31	2.70	1.63	1.55
2	A	435	HYF	C26-C25	3.37	1.56	1.50
2	A	435	HYF	C11-C33	3.45	1.58	1.54
2	A	435	HYF	C29-C28	3.75	1.42	1.35
2	A	435	HYF	C32-C33	4.21	1.60	1.53
2	A	435	HYF	C31-C30	5.27	1.63	1.53
2	A	435	HYF	C31-C18	5.51	1.64	1.52
2	A	435	HYF	C30-C29	6.54	1.61	1.46
2	A	435	HYF	C32-C31	6.74	1.65	1.54
2	A	435	HYF	C34-C33	7.90	1.80	1.56
2	A	435	HYF	C27-C18	10.56	1.70	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	435	HYF	C34-C27-C18	-7.50	96.74	105.01
2	A	435	HYF	C12-C34-C33	-4.96	100.39	110.25
2	A	435	HYF	C32-C33-C11	-4.41	102.03	110.68
2	A	435	HYF	C12-C34-C35	-2.47	103.13	109.26
2	A	435	HYF	C26-C25-C24	2.16	134.57	127.13
2	A	435	HYF	C17-C31-C18	2.31	116.95	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	435	HYF	C36-C35-C34	4.16	124.77	116.48
2	A	435	HYF	C34-C27-C7	4.93	124.27	115.50
2	A	435	HYF	C31-C17-C16	5.17	124.25	113.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	435	HYF	C18-C27-C7-C5
2	A	435	HYF	O8-C7-C27-C18

There are no ring outliers.

1 monomer is involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	435	HYF	28	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

6.1 Protein, DNA and RNA chains

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	273/316 (86%)	0.47	27 (9%) 8 11	16, 35, 81, 89	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	TRP	8.0
1	A	209	LEU	8.0
1	A	312	ALA	7.0
1	A	311	THR	6.8
1	A	207	CYS	6.1
1	A	234	LYS	5.2
1	A	231	SER	5.0
1	A	232	GLY	4.5
1	A	206	LEU	3.3
1	A	229	ALA	3.1
1	A	359	HIS	2.8
1	A	230	ASP	2.8
1	A	315	PHE	2.8
1	A	200	SER	2.7
1	A	236	ILE	2.7
1	A	233	GLY	2.7
1	A	318	LEU	2.6
1	A	310	ASP	2.6
1	A	313	GLY	2.5
1	A	352	ASP	2.5
1	A	202	VAL	2.5
1	A	198	LYS	2.2
1	A	205	ASP	2.2
1	A	360	ARG	2.2
1	A	407	HIS	2.1
1	A	177	VAL	2.1
1	A	295	GLU	2.1

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
2	HYF	A	435	39/39	0.71	0.37	2.53	64,70,75,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.