



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2017 – 03:49 PM EDT

PDB ID : 3IXP
Title : Crystal structure of the ecdysone receptor bound to BYI08346
Authors : Moras, D.; Billas, I.M.L.; Browning, C.
Deposited on : unknown
Resolution : 2.85 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
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)	:	rb-20030345

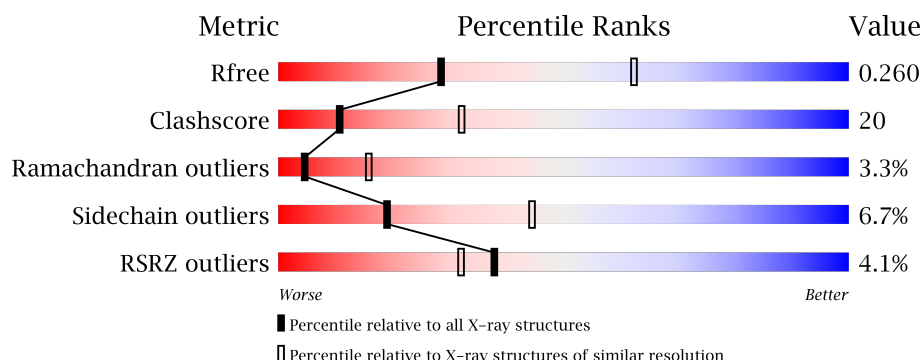
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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	263	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 26%, green 60%, grey 8%);"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%; text-align: center;"> </div> </div> </div>
2	D	265	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 5%, yellow 31%, green 47%, grey 17%);"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%; text-align: center;"> </div> </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
3	EPH	A	900	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3811 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 Gene regulation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1933	1240	338	343	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	MET	-	EXPRESSION TAG	UNP Q7SIF6

- Molecule 2 is a protein called Ecdysone receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	220	Total	C	N	O	S	0	0	0
			1752	1123	295	320	14			

There are 21 discrepancies between the modelled and reference sequences:

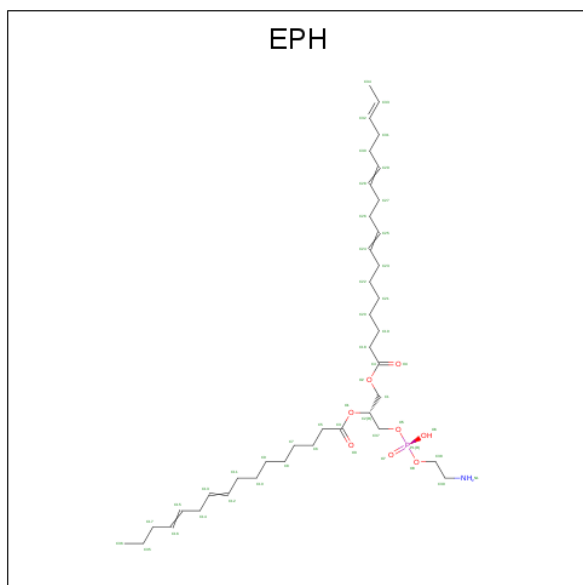
Chain	Residue	Modelled	Actual	Comment	Reference
D	268	GLY	-	EXPRESSION TAG	UNP B9UCQ4
D	269	SER	-	EXPRESSION TAG	UNP B9UCQ4
D	270	HIS	-	EXPRESSION TAG	UNP B9UCQ4
D	271	MET	-	EXPRESSION TAG	UNP B9UCQ4
D	272	ALA	-	EXPRESSION TAG	UNP B9UCQ4
D	273	SER	-	EXPRESSION TAG	UNP B9UCQ4
D	274	MET	-	EXPRESSION TAG	UNP B9UCQ4
D	275	THR	-	EXPRESSION TAG	UNP B9UCQ4
D	276	GLY	-	EXPRESSION TAG	UNP B9UCQ4
D	277	GLY	-	EXPRESSION TAG	UNP B9UCQ4
D	278	GLN	-	EXPRESSION TAG	UNP B9UCQ4
D	279	GLN	-	EXPRESSION TAG	UNP B9UCQ4
D	280	MET	-	EXPRESSION TAG	UNP B9UCQ4
D	281	GLY	-	EXPRESSION TAG	UNP B9UCQ4
D	282	ARG	-	EXPRESSION TAG	UNP B9UCQ4

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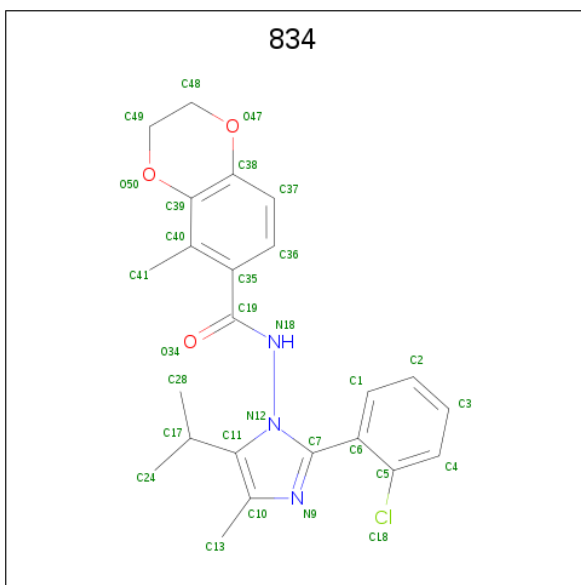
Chain	Residue	Modelled	Actual	Comment	Reference
D	283	ASP	-	EXPRESSION TAG	UNP B9UCQ4
D	284	PRO	-	EXPRESSION TAG	UNP B9UCQ4
D	303	TYR	TRP	ENGINEERED	UNP B9UCQ4
D	361	SER	ALA	ENGINEERED	UNP B9UCQ4
D	456	SER	LEU	ENGINEERED	UNP B9UCQ4
D	483	SER	CYS	ENGINEERED	UNP B9UCQ4

- Molecule 3 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 4 is N-[2-(2-chlorophenyl)-4-methyl-5-(1-methylethyl)-1H-imidazol-1-yl]-5-methyl-2,3-dihydro-1,4-benzodioxine-6-carboxamide (three-letter code: 834) (formula: $C_{23}H_{24}ClN_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	Cl	N	O	
			30	23	1	3	3	
							0	0

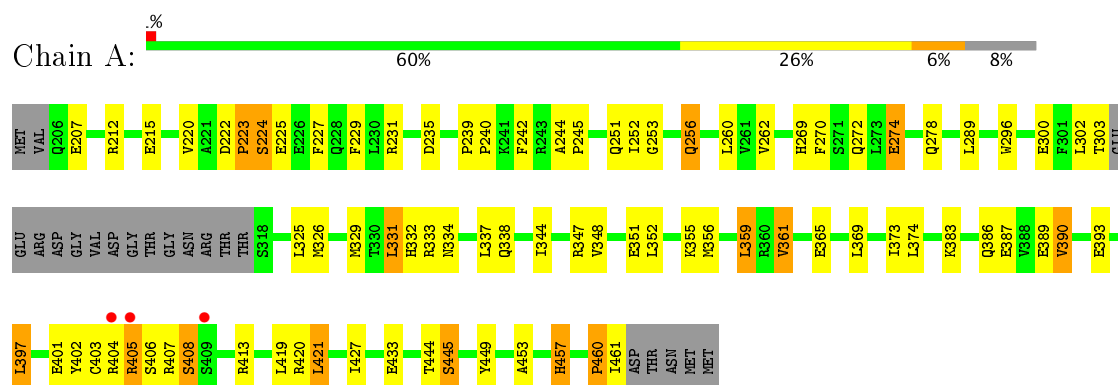
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O		
			27	27	0	0
5	D	20	Total	O		
			20	20	0	0

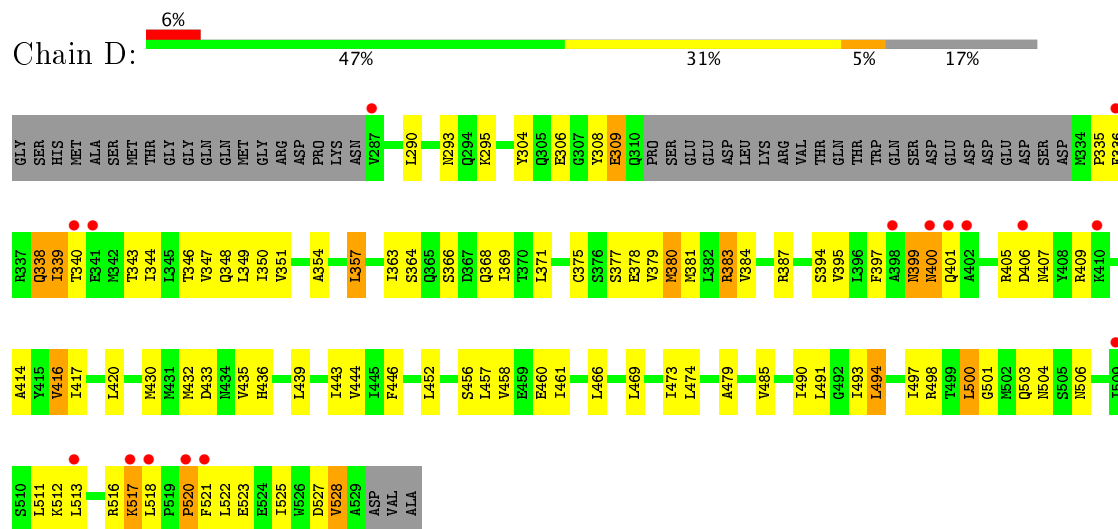
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Gene regulation protein



• Molecule 2: Ecdysone receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.88 Å 147.88 Å 59.78 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.85 48.40 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.85) 100.0 (48.40-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.05 (at 2.86 Å)	Xtriage
Refinement program	REFMAC, CNS 1.1	Depositor
R, R_{free}	0.221 , 0.271 0.216 , 0.260	Depositor DCC
R_{free} test set	1753 reflections (10.92%)	DCC
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3811	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: 834, EPH

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	0.38	0/1971	0.62	0/2662
2	D	0.38	0/1783	0.59	0/2413
All	All	0.38	0/3754	0.60	0/5075

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	1933	0	1976	63	1
2	D	1752	0	1780	94	0
3	A	49	0	67	1	0
4	D	30	0	24	4	0
5	A	27	0	0	2	0
5	D	20	0	0	0	0
All	All	3811	0	3847	155	1

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 20.

The worst 5 of 155 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:274:GLU:HG2	1:A:383:LYS:HD3	1.36	1.05
1:A:326:MET:HG2	1:A:329:MET:HB3	1.49	0.94
2:D:350:ILE:HD13	2:D:379:VAL:HG13	1.56	0.85
1:A:333:ARG:NH1	1:A:337:LEU:HD21	1.95	0.81
2:D:433:ASP:H	2:D:436:HIS:HD2	1.28	0.80

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:MET:CE	1:A:329:MET:CE[6_556]	2.00	0.20

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	238/263 (90%)	210 (88%)	21 (9%)	7 (3%)	5	18
2	D	216/265 (82%)	190 (88%)	18 (8%)	8 (4%)	4	13
All	All	454/528 (86%)	400 (88%)	39 (9%)	15 (3%)	4	16

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	PRO
1	A	224	SER
1	A	408	SER
2	D	309	GLU
2	D	339	ILE

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	212/232 (91%)	195 (92%)	17 (8%)	14	35
2	D	193/235 (82%)	183 (95%)	10 (5%)	27	57
All	All	405/467 (87%)	378 (93%)	27 (7%)	19	44

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	ARG
1	A	433	GLU
2	D	494	LEU
1	A	420	ARG
1	A	272	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	338	GLN
2	D	368	GLN
2	D	436	HIS
1	A	384	ASN
2	D	400	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	$\# Z > 2$
3	EPH	A	900	-	48,48,48	1.87	12 (25%)	50,53,53	2.16	5 (10%)
4	834	D	800	-	29,33,33	1.92	11 (37%)	37,48,48	2.31	10 (27%)

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
3	EPH	A	900	-	-	0/52/52/52	0/0/0/0
4	834	D	800	-	-	0/14/23/23	0/4/4/4

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	EPH	C1-C2	-4.40	1.38	1.50
3	A	900	EPH	C22-C23	-3.04	1.40	1.52
3	A	900	EPH	C20-C19	-2.94	1.34	1.51
3	A	900	EPH	C21-C20	-2.93	1.34	1.51
3	A	900	EPH	P1-O8	-2.06	1.50	1.59

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	EPH	O8-P1-O7	-12.15	60.23	109.25
4	D	800	834	C36-C35-C19	-2.50	111.54	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	800	834	C10-C11-N12	-2.39	104.24	107.02
3	A	900	EPH	C14-C13-C12	-2.35	111.01	124.90
3	A	900	EPH	O6-P1-O8	-2.25	97.54	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	EPH	1	0
4	D	800	834	4	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	242/263 (92%)	-0.19	3 (1%) 79 77	26, 44, 77, 92	0
2	D	220/265 (83%)	0.23	16 (7%) 16 11	27, 53, 88, 97	0
All	All	462/528 (87%)	0.01	19 (4%) 38 32	26, 48, 85, 97	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	400	ASN	5.3
2	D	401	GLN	4.0
1	A	405	ARG	3.8
2	D	410	LYS	3.4
2	D	517	LYS	3.2

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
3	EPH	A	900	49/49	0.82	0.36	7.60	64,73,92,93	0
4	834	D	800	30/30	0.93	0.24	0.18	43,50,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.