



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 02:31 am GMT

PDB ID : 5G0I
Title : Crystal structure of Danio rerio HDAC6 CD1 and CD2 (linker cleaved) in complex with Nexturastat A
Authors : Miyake, Y.; Keusch, J.J.; Wang, L.; Saito, M.; Hess, D.; Wang, X.; Melancon, B.J.; Helquist, P.; Gut, H.; Matthias, P.
Deposited on : 2016-03-18
Resolution : 1.99 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

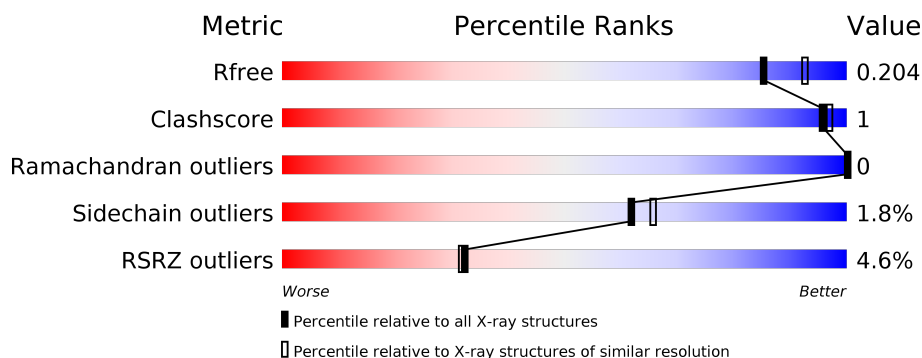
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (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	809	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 7%; height: 10px; background-color: red;"></div> <div style="width: 78%; height: 10px; background-color: green;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> </div> <div> </div> <div> </div> </div>
1	B	809	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 7%; height: 10px; background-color: red;"></div> <div style="width: 77%; height: 10px; background-color: green;"></div> <div style="width: 16%; height: 10px; background-color: yellow;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> </div> <div> </div> <div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12028 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 HDAC6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	722	Total	C	N	O	S	0	4	0
			5653	3569	988	1058	38			
1	B	720	Total	C	N	O	S	0	3	0
			5624	3553	981	1052	38			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP F8W4B7
A	24	PRO	-	expression tag	UNP F8W4B7
B	23	GLY	-	expression tag	UNP F8W4B7
B	24	PRO	-	expression tag	UNP F8W4B7

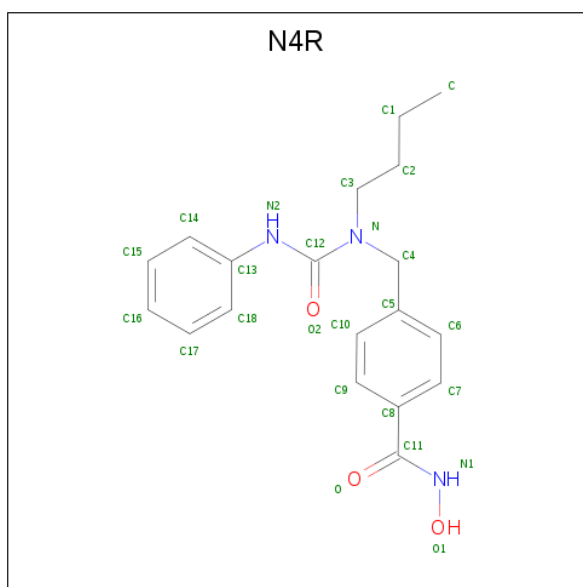
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	K	0	0
			4	4		
3	A	4	Total	K	0	0
			4	4		

- Molecule 4 is NEXTURASTAT A (three-letter code: N4R) (formula: C₁₉H₂₃N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	19	3	3		
4	A	1	Total	C	N	O	0	0
			25	19	3	3		
4	B	1	Total	C	N	O	0	0
			25	19	3	3		
4	B	1	Total	C	N	O	0	0
			25	19	3	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

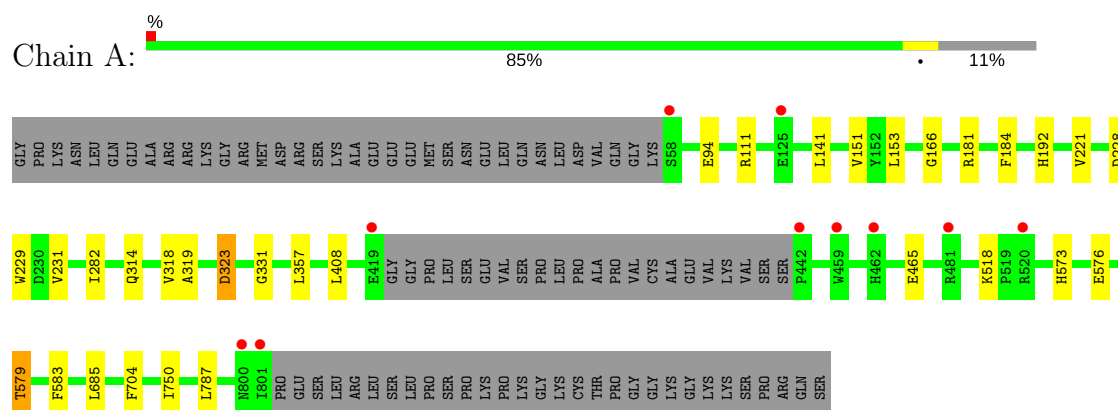
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	425	Total	O	0	0
			425	425		
7	B	205	Total	O	0	0
			205	205		

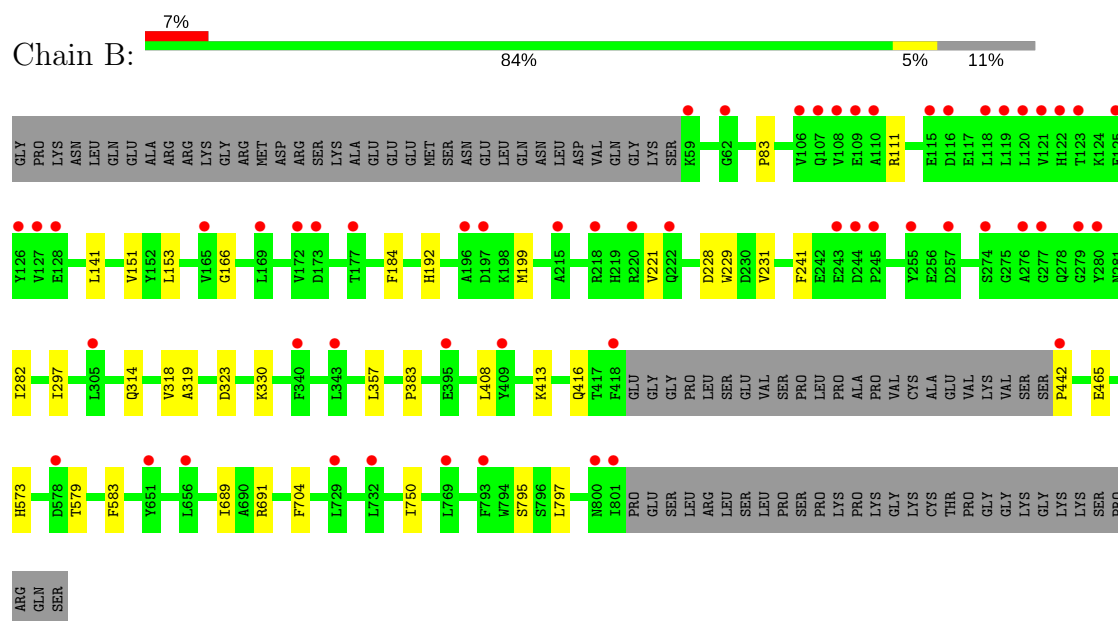
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: HDAC6



• Molecule 1: HDAC6



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.56Å 52.83Å 186.42Å 90.00° 108.92° 90.00°	Depositor
Resolution (Å)	45.58 – 1.99 45.58 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.58-1.99) 98.9 (45.58-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.174 , 0.200 0.175 , 0.204	Depositor DCC
R_{free} test set	5080 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.7	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	0.97	EDS
Total number of atoms	12028	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: ZN, N4R, EDO, K, 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	0.55	0/5792	0.64	0/7856
1	B	0.49	0/5763	0.63	0/7818
All	All	0.52	0/11555	0.64	0/15674

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	5653	0	5498	11	0
1	B	5624	0	5472	15	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	50	0	0	0	0
4	B	50	0	0	0	0
5	A	1	0	0	0	0
6	A	4	0	6	1	0
6	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	425	0	0	0	0
7	B	205	0	0	1	0
All	All	12028	0	10982	26	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 1.

All (26) 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:B:241:PHE:HB3	7:B:2068:HOH:O	1.75	0.85
1:B:297:ILE:HG21	1:B:691:ARG:HD3	1.61	0.81
1:B:297:ILE:HG21	1:B:691:ARG:CD	2.20	0.71
1:B:221:VAL:HG13	1:B:314:GLN:HB2	1.89	0.55
1:B:151:VAL:HG21	1:B:199:MET:HB3	1.90	0.54
1:B:383:PRO:HD3	1:B:442:PRO:HG3	1.90	0.54
1:A:221:VAL:HG13	1:A:314:GLN:HB2	1.93	0.50
1:A:685:LEU:HD21	1:A:787:LEU:HG	1.94	0.48
1:A:111:ARG:O	1:A:166:GLY:HA3	2.14	0.48
1:B:111:ARG:O	1:B:166:GLY:HA3	2.14	0.48
1:B:83:PRO:HG3	1:B:330:LYS:HE3	1.96	0.48
1:B:413:LYS:HA	1:B:416:GLN:HG3	1.96	0.47
1:A:181:ARG:CZ	6:A:1811:EDO:H11	2.45	0.46
1:B:704:PHE:HB2	1:B:750:ILE:HG22	1.97	0.46
1:B:141:LEU:HD22	1:B:153:LEU:HB3	1.98	0.45
1:B:689:ILE:HD11	1:B:797:LEU:HD11	1.99	0.45
1:A:318:VAL:HB	1:A:357:LEU:HG	1.99	0.45
1:A:704:PHE:HB2	1:A:750:ILE:HG22	1.99	0.45
1:A:141:LEU:HD22	1:A:153:LEU:HB3	1.98	0.44
1:B:318:VAL:HB	1:B:357:LEU:HG	1.99	0.43
1:B:282:ILE:HG12	1:B:408:LEU:HG	2.01	0.42
1:A:228:ASP:HA	1:A:319:ALA:HB3	2.02	0.42
1:A:576:GLU:HB2	1:A:579:THR:HG22	2.02	0.42
1:A:282:ILE:HG12	1:A:408:LEU:HG	2.03	0.41
1:B:228:ASP:HA	1:B:319:ALA:HB3	2.02	0.40
1:A:323:ASP:O	1:A:331:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	722/809 (89%)	704 (98%)	18 (2%)	0	100	100
1	B	719/809 (89%)	701 (98%)	18 (2%)	0	100	100
All	All	1441/1618 (89%)	1405 (98%)	36 (2%)	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	615/685 (90%)	603 (98%)	12 (2%)	58	61
1	B	612/685 (89%)	602 (98%)	10 (2%)	65	70
All	All	1227/1370 (90%)	1205 (98%)	22 (2%)	62	66

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	A	151	VAL
1	A	184	PHE
1	A	192	HIS
1	A	229	TRP
1	A	231	VAL
1	A	323	ASP
1	A	465	GLU

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Mol	Chain	Res	Type
1	A	518	LYS
1	A	573	HIS
1	A	579	THR
1	A	583	PHE
1	B	184	PHE
1	B	192	HIS
1	B	229	TRP
1	B	231	VAL
1	B	323	ASP
1	B	465	GLU
1	B	573	HIS
1	B	579	THR
1	B	583	PHE
1	B	795	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 19 ligands modelled in this entry, 13 are monoatomic - leaving 6 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
4	N4R	A	1808	2	26,26,26	0.26	0	32,33,33	0.50	0
4	N4R	A	1809	2	26,26,26	0.28	0	32,33,33	0.64	1 (3%)
6	EDO	A	1811	-	3,3,3	0.47	0	2,2,2	0.22	0
4	N4R	B	1808	2	26,26,26	0.24	0	32,33,33	0.65	1 (3%)
4	N4R	B	1809	2	26,26,26	0.27	0	32,33,33	0.70	1 (3%)
6	EDO	B	1810	-	3,3,3	0.66	0	2,2,2	0.44	0

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
4	N4R	A	1808	2	-	0/22/22/22	0/2/2/2
4	N4R	A	1809	2	-	0/22/22/22	0/2/2/2
6	EDO	A	1811	-	-	0/1/1/1	0/0/0/0
4	N4R	B	1808	2	-	0/22/22/22	0/2/2/2
4	N4R	B	1809	2	-	0/22/22/22	0/2/2/2
6	EDO	B	1810	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1809	N4R	N2-C12-N	-2.17	113.23	115.82
4	B	1808	N4R	N2-C12-N	-2.06	113.36	115.82
4	A	1809	N4R	C3-N-C12	2.21	128.35	120.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1811	EDO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	722/809 (89%)	-0.08	10 (1%) 75 74	30, 41, 66, 113	0
1	B	720/809 (88%)	0.33	56 (7%) 13 12	36, 61, 105, 183	0
All	All	1442/1618 (89%)	0.12	66 (4%) 32 32	30, 49, 95, 183	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	801	ILE	7.3
1	A	801	ILE	5.3
1	B	220	ARG	4.9
1	B	119	LEU	4.9
1	A	800	ASN	4.5
1	B	125	GLU	4.2
1	B	279	GLY	4.2
1	B	121	VAL	4.1
1	A	442	PRO	4.0
1	B	442	PRO	3.9
1	A	58	SER	3.7
1	B	126	TYR	3.7
1	B	215	ALA	3.7
1	B	165	VAL	3.7
1	B	120	LEU	3.6
1	A	520	ARG	3.6
1	B	274	SER	3.5
1	B	276	ALA	3.5
1	B	409	TYR	3.4
1	A	419	GLU	3.4
1	B	800	ASN	3.4
1	B	116	ASP	3.3
1	B	418	PHE	3.3
1	B	115	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	123	THR	3.1
1	B	107	GLN	3.1
1	B	656	LEU	3.0
1	B	277	GLY	2.9
1	B	127	VAL	2.9
1	B	118	LEU	2.8
1	B	108	VAL	2.8
1	B	169	LEU	2.7
1	B	769	LEU	2.6
1	B	255	TYR	2.6
1	B	245	PRO	2.5
1	A	481	ARG	2.5
1	B	197	ASP	2.5
1	B	343	LEU	2.5
1	B	578	ASP	2.4
1	B	793	PHE	2.4
1	B	244	ASP	2.4
1	B	128	GLU	2.4
1	A	462	HIS	2.4
1	B	177	THR	2.3
1	B	109	GLU	2.3
1	B	218	ARG	2.3
1	B	651	TYR	2.2
1	B	732	LEU	2.2
1	B	110	ALA	2.2
1	B	106	VAL	2.2
1	B	172	VAL	2.2
1	B	280	TYR	2.1
1	A	125	GLU	2.1
1	B	243	GLU	2.1
1	B	59	LYS	2.1
1	B	196	ALA	2.1
1	B	257	ASP	2.1
1	B	62	GLY	2.1
1	B	305	LEU	2.1
1	B	122	HIS	2.0
1	B	729	LEU	2.0
1	B	340	PHE	2.0
1	A	459	TRP	2.0
1	B	173	ASP	2.0
1	B	222	GLN	2.0
1	B	395	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 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. 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(\AA^2)	Q<0.9
5	CL	A	1810	1/1	0.70	0.10	104,104,104,104	0
4	N4R	B	1809	25/25	0.85	0.19	57,71,82,85	0
4	N4R	B	1808	25/25	0.89	0.17	64,72,79,80	0
3	K	B	1804	1/1	0.89	0.09	55,55,55,55	0
4	N4R	A	1808	25/25	0.90	0.15	48,57,69,71	0
4	N4R	A	1809	25/25	0.92	0.13	48,55,64,68	0
3	K	B	1806	1/1	0.93	0.07	49,49,49,49	0
6	EDO	A	1811	4/4	0.95	0.12	42,48,51,52	0
6	EDO	B	1810	4/4	0.96	0.17	48,51,51,52	0
2	ZN	B	1802	1/1	0.97	0.11	44,44,44,44	1
3	K	B	1805	1/1	0.97	0.10	52,52,52,52	0
2	ZN	B	1803	1/1	0.98	0.10	45,45,45,45	1
3	K	A	1806	1/1	0.99	0.09	35,35,35,35	0
3	K	B	1807	1/1	0.99	0.07	70,70,70,70	0
3	K	A	1807	1/1	0.99	0.10	38,38,38,38	0
2	ZN	A	1802	1/1	1.00	0.10	41,41,41,41	1
2	ZN	A	1803	1/1	1.00	0.11	39,39,39,39	1
3	K	A	1804	1/1	1.00	0.10	34,34,34,34	0
3	K	A	1805	1/1	1.00	0.14	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.