



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:54 pm GMT

PDB ID : 4BB5  
Title : Free-Wilson and Structural Approaches to Co-optimising Human and Rodent Isoform Potency for 11b-Hydroxysteroid Dehydrogenase Type 1 11b-HSD1 Inhibitors  
Authors : Goldberg, F.W.; Leach, A.G.; Scott, J.S.; Snelson, W.L.; Groombridge, S.D.; Donald, C.S.; Bennett, S.N.L.; Bodin, C.; Morentin Gutierrez, P.; Gyte, A.C.  
Deposited on : 2012-09-20  
Resolution : 2.20 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](mailto: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.

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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

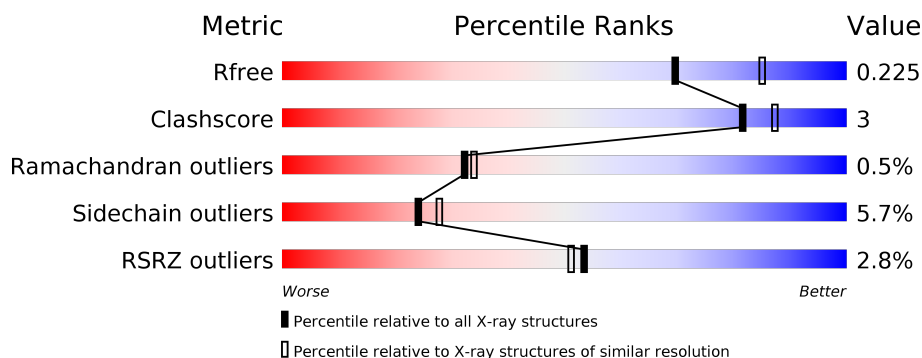
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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  $\geq 3$ , 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	292	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>10%</div> </div> </div>
1	B	292	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>10%</div> </div> </div>
1	C	292	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>13%</div> </div> </div>
1	D	292	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8641 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 CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2023	1288	346	374	15			
1	B	264	Total	C	N	O	S	0	0	0
			2032	1293	347	377	15			
1	C	254	Total	C	N	O	S	0	0	0
			1943	1237	333	359	14			
1	D	262	Total	C	N	O	S	0	0	0
			2015	1282	343	375	15			

There are 16 discrepancies between the modelled and reference sequences:

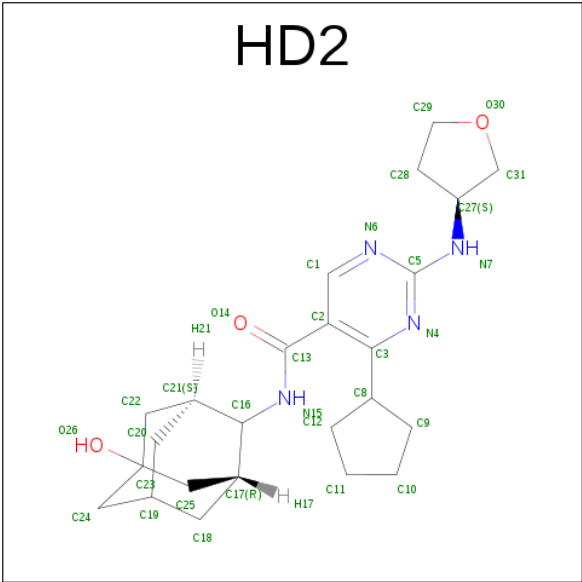
Chain	Residue	Modelled	Actual	Comment	Reference
A	179	LEU	MET	CONFLICT	UNP P28845
A	262	ARG	LEU	CONFLICT	UNP P28845
A	272	SER	CYS	CONFLICT	UNP P28845
A	278	GLU	PHE	CONFLICT	UNP P28845
B	179	LEU	MET	CONFLICT	UNP P28845
B	262	ARG	LEU	CONFLICT	UNP P28845
B	272	SER	CYS	CONFLICT	UNP P28845
B	278	GLU	PHE	CONFLICT	UNP P28845
C	179	LEU	MET	CONFLICT	UNP P28845
C	262	ARG	LEU	CONFLICT	UNP P28845
C	272	SER	CYS	CONFLICT	UNP P28845
C	278	GLU	PHE	CONFLICT	UNP P28845
D	179	LEU	MET	CONFLICT	UNP P28845
D	262	ARG	LEU	CONFLICT	UNP P28845
D	272	SER	CYS	CONFLICT	UNP P28845
D	278	GLU	PHE	CONFLICT	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 4-CYCLOPENTYL-N-[(1S,3R)-5-OXIDANYL-2-ADAMANTYL]-2-[[[(3S)-OXOLAN-3-YL]AMINO]PYRIMIDINE-5-CARBOXAMIDE (three-letter code: HD2) (formula: C<sub>24</sub>H<sub>34</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	24	4	3		
3	B	1	Total	C	N	O	0	0
			31	24	4	3		
3	C	1	Total	C	N	O	0	0
			31	24	4	3		
3	D	1	Total	C	N	O	0	0
			31	24	4	3		

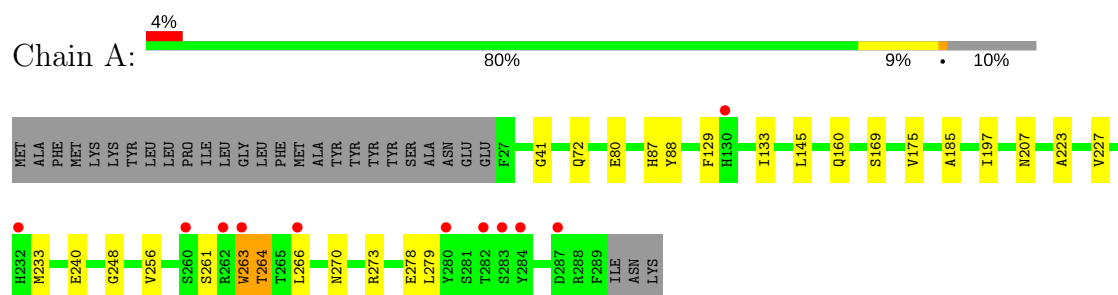
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total	O	0	0
			98	98		
4	B	89	Total	O	0	0
			89	89		
4	C	90	Total	O	0	0
			90	90		
4	D	35	Total	O	0	0
			35	35		

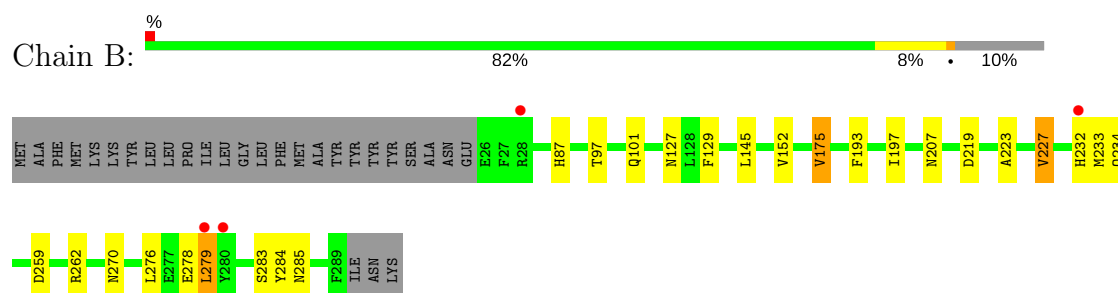
### 3 Residue-property plots [i](#)

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.

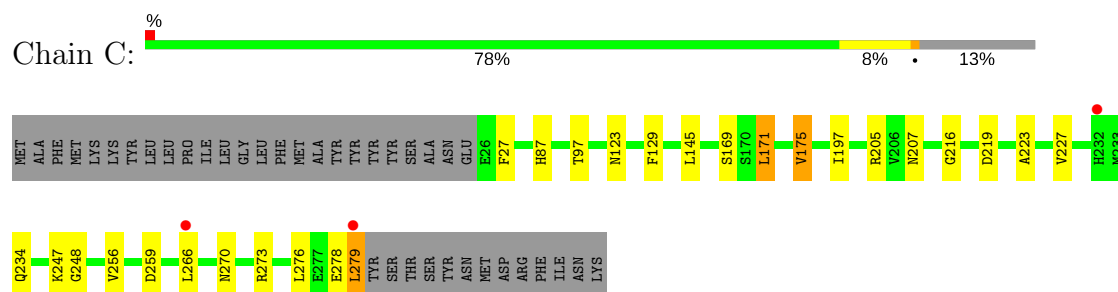
#### • Molecule 1: CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1



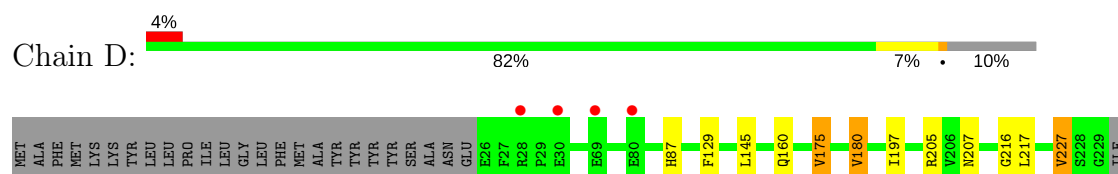
#### • Molecule 1: CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1

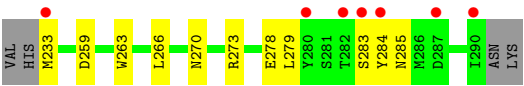


#### • Molecule 1: CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1



#### • Molecule 1: CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.78Å 132.48Å 154.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.20 34.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.00-2.20) 99.6 (34.25-2.20)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.22 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, $R_{free}$	0.182 , 0.220 0.184 , 0.225	Depositor DCC
$R_{free}$ test set	2607 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8641	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAP, HD2

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	0/2057	0.67	0/2776
1	B	0.50	0/2066	0.67	0/2788
1	C	0.49	0/1974	0.66	0/2664
1	D	0.47	0/2047	0.65	0/2760
All	All	0.49	0/8144	0.67	0/10988

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	2023	0	2070	19	0
1	B	2032	0	2076	15	0
1	C	1943	0	2000	19	0
1	D	2015	0	2059	15	0
2	A	48	0	25	2	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0
3	A	31	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	34	1	0
3	C	31	0	34	1	0
3	D	31	0	34	2	0
4	A	98	0	0	1	0
4	B	89	0	0	1	0
4	C	90	0	0	1	0
4	D	35	0	0	1	0
All	All	8641	0	8441	50	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 3.

All (50) 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:87:HIS:HD2	4:A:2007:HOH:O	1.79	0.66
1:C:129:PHE:HB3	1:D:197:ILE:HD11	1.79	0.64
1:D:216:GLY:HA3	1:D:259:ASP:OD1	1.97	0.64
1:C:197:ILE:HD11	1:D:129:PHE:HB3	1.79	0.63
1:A:197:ILE:HD11	1:B:129:PHE:HB3	1.81	0.61
1:A:129:PHE:HB3	1:B:197:ILE:HD11	1.85	0.58
3:A:1291:HD2:N4	3:A:1291:HD2:H281	2.22	0.54
1:C:129:PHE:HB3	1:D:197:ILE:CD1	2.37	0.54
1:C:197:ILE:CD1	1:D:129:PHE:HB3	2.37	0.54
1:D:87:HIS:HD2	4:D:2004:HOH:O	1.90	0.54
1:B:87:HIS:HD2	4:B:2014:HOH:O	1.90	0.53
3:D:1292:HD2:H281	3:D:1292:HD2:N4	2.25	0.51
1:C:216:GLY:HA3	1:C:259:ASP:OD1	2.12	0.50
1:A:273:ARG:HG3	1:B:175:VAL:HG22	1.94	0.50
1:C:171:LEU:HD22	1:C:216:GLY:HA2	1.94	0.49
1:A:72:GLN:HG3	1:A:88:TYR:CE2	2.47	0.49
1:B:101:GLN:HG3	1:C:123:ASN:OD1	2.13	0.49
1:A:129:PHE:HB3	1:B:197:ILE:CD1	2.43	0.48
1:A:223:ALA:O	1:A:227:VAL:HB	2.14	0.48
1:A:263:TRP:HE1	1:B:279:LEU:CD2	2.26	0.48
3:A:1291:HD2:H291	1:B:284:TYR:CE1	2.49	0.47
1:C:223:ALA:O	1:C:227:VAL:HB	2.14	0.47
1:D:217:LEU:HD21	1:D:227:VAL:HG11	1.96	0.47
1:A:197:ILE:CD1	1:B:129:PHE:HB3	2.45	0.47
1:C:197:ILE:HD11	1:D:129:PHE:CB	2.45	0.46
1:A:264:THR:HB	1:B:276:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:SER:HB3	1:A:264:THR:HG23	1.98	0.46
3:B:1291:HD2:N4	3:B:1291:HD2:H281	2.32	0.45
1:A:248:GLY:HA3	1:A:256:VAL:HG21	1.98	0.45
1:B:223:ALA:O	1:B:227:VAL:HB	2.17	0.45
1:C:169:SER:O	2:C:1280:NAP:H6N	2.17	0.45
1:C:175:VAL:HG22	1:D:273:ARG:HG3	1.99	0.44
1:C:273:ARG:HG3	1:D:175:VAL:HG22	2.00	0.44
1:C:129:PHE:CB	1:D:197:ILE:HD11	2.46	0.44
1:A:248:GLY:HA3	1:A:256:VAL:CG2	2.46	0.44
1:C:279:LEU:HD21	1:D:263:TRP:HE3	1.83	0.43
1:D:180:VAL:HG21	3:D:1292:HD2:H122	2.00	0.43
1:A:263:TRP:HE1	1:B:279:LEU:HD21	1.83	0.43
1:C:248:GLY:HA3	1:C:256:VAL:HG21	2.02	0.42
1:A:169:SER:O	2:A:1290:NAP:H6N	2.20	0.42
1:A:185:ALA:HB2	1:B:193:PHE:HB2	2.02	0.42
1:C:248:GLY:HA3	1:C:256:VAL:CG2	2.49	0.42
1:C:87:HIS:HD2	4:C:2018:HOH:O	2.03	0.42
3:C:1281:HD2:H291	1:D:284:TYR:CE1	2.54	0.42
1:C:276:LEU:HD23	1:D:175:VAL:HG21	2.01	0.41
1:A:41:GLY:HA2	2:A:1290:NAP:H1B	2.01	0.41
1:A:263:TRP:CD1	1:A:263:TRP:C	2.93	0.41
1:A:133:ILE:HD11	1:B:152:VAL:HG21	2.02	0.41
1:C:27:PHE:CD2	1:C:247:LYS:HG2	2.56	0.41
1:B:232:HIS:N	1:B:232:HIS:CD2	2.89	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	261/292 (89%)	250 (96%)	11 (4%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	262/292 (90%)	251 (96%)	8 (3%)	3 (1%)	17	13
1	C	252/292 (86%)	243 (96%)	8 (3%)	1 (0%)	38	41
1	D	258/292 (88%)	247 (96%)	10 (4%)	1 (0%)	38	41
All	All	1033/1168 (88%)	991 (96%)	37 (4%)	5 (0%)	32	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	MET
1	D	283	SER
1	B	219	ASP
1	B	283	SER
1	C	219	ASP

### 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	220/245 (90%)	207 (94%)	13 (6%)	23	26
1	B	221/245 (90%)	208 (94%)	13 (6%)	23	26
1	C	211/245 (86%)	200 (95%)	11 (5%)	27	32
1	D	219/245 (89%)	206 (94%)	13 (6%)	23	26
All	All	871/980 (89%)	821 (94%)	50 (6%)	24	28

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	145	LEU
1	A	160	GLN
1	A	175	VAL
1	A	207	ASN
1	A	233	MET

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Mol	Chain	Res	Type
1	A	240	GLU
1	A	263	TRP
1	A	264	THR
1	A	266	LEU
1	A	270	ASN
1	A	278	GLU
1	A	279	LEU
1	B	97	THR
1	B	127	ASN
1	B	145	LEU
1	B	175	VAL
1	B	207	ASN
1	B	227	VAL
1	B	234	GLN
1	B	259	ASP
1	B	262	ARG
1	B	270	ASN
1	B	278	GLU
1	B	279	LEU
1	B	285	ASN
1	C	97	THR
1	C	145	LEU
1	C	171	LEU
1	C	175	VAL
1	C	205	ARG
1	C	207	ASN
1	C	234	GLN
1	C	266	LEU
1	C	270	ASN
1	C	278	GLU
1	C	279	LEU
1	D	145	LEU
1	D	160	GLN
1	D	175	VAL
1	D	180	VAL
1	D	205	ARG
1	D	207	ASN
1	D	227	VAL
1	D	233	MET
1	D	266	LEU
1	D	270	ASN
1	D	278	GLU

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Mol	Chain	Res	Type
1	D	279	LEU
1	D	285	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	87	HIS
1	A	105	GLN
1	A	123	ASN
1	A	127	ASN
1	A	207	ASN
1	A	270	ASN
1	B	87	HIS
1	B	123	ASN
1	B	127	ASN
1	B	207	ASN
1	B	232	HIS
1	B	270	ASN
1	C	77	HIS
1	C	87	HIS
1	C	101	GLN
1	C	127	ASN
1	C	160	GLN
1	C	207	ASN
1	C	270	ASN
1	D	77	HIS
1	D	87	HIS
1	D	101	GLN
1	D	123	ASN
1	D	127	ASN
1	D	207	ASN
1	D	270	ASN

### 5.3.3 RNA ⓘ

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](#)

8 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$
2	NAP	A	1290	-	44,52,52	3.09	15 (34%)	51,80,80	2.81	23 (45%)
3	HD2	A	1291	-	36,36,36	0.98	2 (5%)	37,54,54	1.86	6 (16%)
2	NAP	B	1290	-	44,52,52	3.58	18 (40%)	51,80,80	3.25	28 (54%)
3	HD2	B	1291	-	36,36,36	1.06	1 (2%)	37,54,54	1.46	5 (13%)
2	NAP	C	1280	-	44,52,52	3.08	16 (36%)	51,80,80	3.04	26 (50%)
3	HD2	C	1281	-	36,36,36	1.03	2 (5%)	37,54,54	1.60	8 (21%)
2	NAP	D	1291	-	44,52,52	3.16	19 (43%)	51,80,80	3.33	27 (52%)
3	HD2	D	1292	-	36,36,36	0.99	2 (5%)	37,54,54	1.62	7 (18%)

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	NAP	A	1290	-	-	0/27/67/67	0/5/5/5
3	HD2	A	1291	-	-	0/14/61/61	0/3/6/6
2	NAP	B	1290	-	-	0/27/67/67	0/5/5/5
3	HD2	B	1291	-	-	0/14/61/61	0/3/6/6
2	NAP	C	1280	-	-	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HD2	C	1281	-	-	0/14/61/61	0/3/6/6
2	NAP	D	1291	-	-	0/27/67/67	0/5/5/5
3	HD2	D	1292	-	-	0/14/61/61	0/3/6/6

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1290	NAP	O4B-C1B	-7.89	1.30	1.41
2	D	1291	NAP	O4B-C1B	-6.82	1.31	1.41
2	A	1290	NAP	O4B-C1B	-6.69	1.32	1.41
2	C	1280	NAP	O4B-C1B	-5.77	1.33	1.41
2	B	1290	NAP	C2D-C3D	-5.15	1.39	1.53
2	A	1290	NAP	O7N-C7N	-5.10	1.13	1.24
2	A	1290	NAP	C2D-C3D	-4.84	1.40	1.53
2	B	1290	NAP	O4D-C1D	-4.67	1.34	1.41
2	B	1290	NAP	O7N-C7N	-4.41	1.15	1.24
2	C	1280	NAP	C2D-C3D	-4.21	1.42	1.53
2	D	1291	NAP	O7N-C7N	-4.00	1.15	1.24
2	A	1290	NAP	O4D-C1D	-3.89	1.35	1.41
2	D	1291	NAP	C2D-C3D	-3.82	1.43	1.53
2	D	1291	NAP	O4D-C1D	-3.32	1.36	1.41
2	A	1290	NAP	C5A-N7A	-2.57	1.30	1.39
2	B	1290	NAP	O3B-C3B	-2.46	1.37	1.43
2	B	1290	NAP	C5D-C4D	-2.40	1.44	1.51
2	B	1290	NAP	C3N-C7N	-2.30	1.46	1.50
2	D	1291	NAP	O3B-C3B	-2.27	1.37	1.43
3	D	1292	HD2	C2-C3	-2.27	1.38	1.41
3	C	1281	HD2	C2-C3	-2.23	1.38	1.41
3	A	1291	HD2	C2-C3	-2.14	1.38	1.41
2	C	1280	NAP	PA-O2A	-2.10	1.44	1.55
2	D	1291	NAP	P2B-O1X	2.19	1.58	1.50
2	A	1290	NAP	O4D-C4D	2.34	1.50	1.45
2	C	1280	NAP	O4D-C4D	2.43	1.50	1.45
2	C	1280	NAP	P2B-O2B	2.48	1.63	1.59
2	A	1290	NAP	O2D-C2D	2.52	1.48	1.43
2	D	1291	NAP	C2A-N3A	2.59	1.36	1.32
2	A	1290	NAP	C6A-N1A	2.64	1.49	1.37
2	B	1290	NAP	C7N-N7N	2.66	1.38	1.33
2	B	1290	NAP	O2D-C2D	2.67	1.49	1.43
2	D	1291	NAP	C6N-C5N	2.70	1.44	1.38
2	D	1291	NAP	C7N-N7N	2.71	1.38	1.33
2	C	1280	NAP	C2A-N1A	2.72	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1291	NAP	O4D-C4D	2.78	1.51	1.45
2	C	1280	NAP	C6A-N1A	2.79	1.49	1.37
2	B	1290	NAP	O4D-C4D	2.86	1.51	1.45
2	D	1291	NAP	C6A-N1A	2.93	1.50	1.37
2	B	1290	NAP	C6A-N1A	3.01	1.50	1.37
2	A	1290	NAP	O3D-C3D	3.04	1.50	1.43
2	D	1291	NAP	C4A-N3A	3.10	1.40	1.35
2	C	1280	NAP	C6N-C5N	3.11	1.45	1.38
3	D	1292	HD2	C5-N7	3.50	1.39	1.34
2	B	1290	NAP	C2N-C3N	3.80	1.44	1.39
3	A	1291	HD2	C5-N7	3.85	1.40	1.34
2	A	1290	NAP	C2N-C3N	3.86	1.44	1.39
2	C	1280	NAP	C2N-C3N	3.96	1.45	1.39
2	D	1291	NAP	C2N-C3N	4.12	1.45	1.39
3	C	1281	HD2	C5-N7	4.25	1.41	1.34
3	B	1291	HD2	C5-N7	4.60	1.41	1.34
2	C	1280	NAP	O3D-C3D	4.70	1.53	1.43
2	D	1291	NAP	O3D-C3D	4.97	1.54	1.43
2	D	1291	NAP	C5B-C4B	4.98	1.67	1.51
2	C	1280	NAP	C7N-N7N	5.02	1.42	1.33
2	A	1290	NAP	C5B-C4B	5.12	1.67	1.51
2	C	1280	NAP	C5B-C4B	5.46	1.68	1.51
2	D	1291	NAP	C3D-C4D	5.60	1.67	1.53
2	A	1290	NAP	C3D-C4D	5.88	1.68	1.53
2	C	1280	NAP	C3D-C4D	5.95	1.68	1.53
2	C	1280	NAP	C3B-C4B	6.35	1.69	1.53
2	C	1280	NAP	O4B-C4B	6.37	1.59	1.45
2	B	1290	NAP	C5B-C4B	6.38	1.71	1.51
2	D	1291	NAP	C3B-C4B	6.57	1.70	1.53
2	B	1290	NAP	C3D-C4D	6.65	1.70	1.53
2	B	1290	NAP	O3D-C3D	6.72	1.58	1.43
2	A	1290	NAP	O4B-C4B	6.92	1.60	1.45
2	A	1290	NAP	C3B-C4B	7.09	1.71	1.53
2	B	1290	NAP	O4B-C4B	7.65	1.62	1.45
2	D	1291	NAP	C4N-C3N	7.67	1.52	1.39
2	D	1291	NAP	O4B-C4B	7.81	1.62	1.45
2	B	1290	NAP	C3B-C4B	8.01	1.74	1.53
2	A	1290	NAP	C4N-C3N	8.41	1.53	1.39
2	C	1280	NAP	C4N-C3N	8.59	1.53	1.39
2	B	1290	NAP	C4N-C3N	9.20	1.54	1.39

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1291	NAP	N3A-C2A-N1A	-13.49	117.11	128.86
2	B	1290	NAP	N3A-C2A-N1A	-10.88	119.38	128.86
2	A	1290	NAP	N3A-C2A-N1A	-10.17	120.00	128.86
2	C	1280	NAP	N3A-C2A-N1A	-9.16	120.88	128.86
3	A	1291	HD2	C5-N7-C27	-7.14	115.65	123.56
2	B	1290	NAP	O3B-C3B-C4B	-6.07	93.35	111.09
2	C	1280	NAP	O3B-C3B-C4B	-6.00	93.56	111.09
2	A	1290	NAP	O4B-C1B-C2B	-5.58	96.82	106.59
2	D	1291	NAP	O3B-C3B-C4B	-5.38	95.38	111.09
2	D	1291	NAP	O3D-C3D-C4D	-5.03	96.39	111.09
2	D	1291	NAP	O2X-P2B-O1X	-5.00	90.95	110.50
2	B	1290	NAP	O3D-C3D-C4D	-4.96	96.60	111.09
2	B	1290	NAP	O2X-P2B-O1X	-4.90	91.34	110.50
3	C	1281	HD2	C5-N7-C27	-4.86	118.17	123.56
2	A	1290	NAP	O4B-C4B-C5B	-4.85	93.02	109.40
2	D	1291	NAP	O4B-C1B-C2B	-4.82	98.15	106.59
2	C	1280	NAP	O2X-P2B-O1X	-4.77	91.82	110.50
2	D	1291	NAP	O3X-P2B-O1X	-4.77	91.82	110.50
2	C	1280	NAP	O5B-C5B-C4B	-4.75	92.15	109.00
2	C	1280	NAP	O2B-P2B-O1X	-4.72	90.76	109.26
2	B	1290	NAP	C6N-C5N-C4N	-4.54	112.59	119.44
2	C	1280	NAP	O3D-C3D-C4D	-4.50	97.94	111.09
2	A	1290	NAP	O2X-P2B-O1X	-4.34	93.50	110.50
3	D	1292	HD2	C5-N7-C27	-4.34	118.75	123.56
2	B	1290	NAP	O5B-C5B-C4B	-4.33	93.65	109.00
2	D	1291	NAP	O4B-C4B-C5B	-4.29	94.92	109.40
2	C	1280	NAP	O4B-C4B-C5B	-4.25	95.06	109.40
2	D	1291	NAP	O5B-C5B-C4B	-4.20	94.11	109.00
2	C	1280	NAP	O4B-C1B-C2B	-4.13	99.37	106.59
3	A	1291	HD2	C23-C22-C21	-4.12	108.43	109.87
2	A	1290	NAP	O5B-C5B-C4B	-4.10	94.46	109.00
2	B	1290	NAP	O4B-C4B-C5B	-4.01	95.87	109.40
3	D	1292	HD2	C12-C8-C3	-4.00	108.58	114.38
2	B	1290	NAP	C3N-C2N-N1N	-3.93	116.47	120.43
2	B	1290	NAP	O2B-P2B-O1X	-3.93	93.87	109.26
2	C	1280	NAP	C3N-C7N-N7N	-3.92	113.30	117.77
2	A	1290	NAP	O3B-C3B-C4B	-3.87	99.77	111.09
2	B	1290	NAP	O2B-C2B-C3B	-3.83	97.44	111.63
2	B	1290	NAP	C4D-O4D-C1D	-3.73	105.80	109.77
2	B	1290	NAP	O3X-P2B-O1X	-3.71	96.00	110.50
3	B	1291	HD2	C12-C8-C3	-3.62	109.12	114.38
3	B	1291	HD2	C23-C22-C21	-3.61	108.61	109.87
2	D	1291	NAP	O2B-P2B-O1X	-3.58	95.22	109.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1290	NAP	C1B-N9A-C4A	-3.56	120.48	126.64
2	B	1290	NAP	O4B-C4B-C3B	-3.53	98.15	105.17
2	D	1291	NAP	C6N-C5N-C4N	-3.52	114.13	119.44
2	D	1291	NAP	C1B-N9A-C4A	-3.44	120.69	126.64
2	C	1280	NAP	O2B-C2B-C3B	-3.38	99.09	111.63
2	A	1290	NAP	O3D-C3D-C4D	-3.27	101.54	111.09
3	A	1291	HD2	C12-C8-C3	-3.26	109.65	114.38
3	C	1281	HD2	C23-C22-C21	-3.24	108.73	109.87
2	C	1280	NAP	O3X-P2B-O1X	-3.21	97.93	110.50
2	B	1290	NAP	O4B-C1B-C2B	-3.16	101.07	106.59
2	A	1290	NAP	O2B-P2B-O1X	-3.06	97.25	109.26
2	A	1290	NAP	O7N-C7N-C3N	-3.00	116.12	119.62
2	A	1290	NAP	O2B-C2B-C3B	-2.96	100.67	111.63
2	C	1280	NAP	C1B-N9A-C4A	-2.94	121.55	126.64
2	A	1290	NAP	O3X-P2B-O1X	-2.92	99.09	110.50
3	D	1292	HD2	C9-C8-C3	-2.81	110.30	114.38
2	B	1290	NAP	C2D-C3D-C4D	-2.80	97.16	102.62
2	C	1280	NAP	C3N-C2N-N1N	-2.79	117.61	120.43
3	C	1281	HD2	N6-C5-N4	-2.73	124.05	126.68
2	D	1291	NAP	O2B-C2B-C3B	-2.73	101.52	111.63
2	D	1291	NAP	C5B-C4B-C3B	-2.73	104.89	115.29
2	B	1290	NAP	C5B-C4B-C3B	-2.70	105.00	115.29
2	A	1290	NAP	C6N-C5N-C4N	-2.66	115.42	119.44
3	C	1281	HD2	C12-C8-C3	-2.66	110.52	114.38
3	A	1291	HD2	C2-C13-N15	-2.63	111.87	116.88
2	D	1291	NAP	O4B-C4B-C3B	-2.62	99.96	105.17
2	B	1290	NAP	O7N-C7N-C3N	-2.58	116.60	119.62
2	D	1291	NAP	C3N-C7N-N7N	-2.52	114.90	117.77
2	C	1280	NAP	C6N-C5N-C4N	-2.49	115.69	119.44
2	A	1290	NAP	O4B-C4B-C3B	-2.48	100.24	105.17
2	C	1280	NAP	C4D-O4D-C1D	-2.47	107.14	109.77
3	C	1281	HD2	C2-C13-N15	-2.46	112.20	116.88
2	D	1291	NAP	C4D-O4D-C1D	-2.45	107.16	109.77
3	D	1292	HD2	C2-C13-N15	-2.41	112.30	116.88
2	A	1290	NAP	C5A-C6A-N1A	-2.35	112.60	119.70
2	A	1290	NAP	C4D-O4D-C1D	-2.35	107.27	109.77
2	C	1280	NAP	C5A-C6A-N1A	-2.27	112.82	119.70
2	D	1291	NAP	C3N-C2N-N1N	-2.25	118.16	120.43
2	A	1290	NAP	C2B-C3B-C4B	-2.18	96.99	101.95
3	A	1291	HD2	C9-C8-C3	-2.17	111.23	114.38
3	C	1281	HD2	C9-C8-C3	-2.10	111.33	114.38
2	D	1291	NAP	O2D-C2D-C3D	-2.10	105.11	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1280	NAP	C2B-C3B-C4B	-2.09	97.20	101.95
2	A	1290	NAP	C1B-N9A-C4A	-2.07	123.06	126.64
2	B	1290	NAP	C5A-C6A-N1A	-2.06	113.48	119.70
2	D	1291	NAP	C4A-C5A-N7A	2.07	111.41	109.41
2	B	1290	NAP	O2N-PN-O1N	2.12	123.26	112.28
3	B	1291	HD2	O14-C13-N15	2.14	126.37	122.46
2	D	1291	NAP	C5N-C4N-C3N	2.17	122.90	120.35
3	B	1291	HD2	C12-C8-C9	2.22	106.40	102.28
2	B	1290	NAP	O2X-P2B-O2B	2.28	116.35	106.00
2	C	1280	NAP	O2X-P2B-O2B	2.28	116.36	106.00
2	B	1290	NAP	C5N-C4N-C3N	2.28	123.03	120.35
2	A	1290	NAP	O7N-C7N-N7N	2.29	125.84	122.58
2	D	1291	NAP	C4B-O4B-C1B	2.30	112.22	109.77
2	A	1290	NAP	O2N-PN-O1N	2.34	124.37	112.28
2	B	1290	NAP	O5D-PN-O1N	2.46	119.16	109.25
2	D	1291	NAP	O2X-P2B-O2B	2.60	117.81	106.00
3	A	1291	HD2	C12-C8-C9	2.68	107.26	102.28
3	D	1292	HD2	C28-C27-N7	2.70	117.98	111.98
3	C	1281	HD2	O14-C13-N15	2.75	127.49	122.46
2	C	1280	NAP	O2A-PA-O1A	2.91	127.33	112.28
2	D	1291	NAP	O2N-PN-O1N	2.94	127.48	112.28
2	C	1280	NAP	C5A-C6A-N6A	2.98	126.53	120.47
2	B	1290	NAP	O7N-C7N-N7N	3.11	127.01	122.58
2	D	1291	NAP	O7N-C7N-N7N	3.13	127.03	122.58
2	C	1280	NAP	C5N-C6N-N1N	3.14	125.24	120.40
3	D	1292	HD2	C12-C8-C9	3.15	108.14	102.28
2	C	1280	NAP	O7N-C7N-N7N	3.27	127.23	122.58
2	A	1290	NAP	C5A-C6A-N6A	3.32	127.25	120.47
3	D	1292	HD2	O14-C13-N15	3.33	128.55	122.46
2	B	1290	NAP	C4B-O4B-C1B	3.37	113.35	109.77
2	C	1280	NAP	C2A-N1A-C6A	3.43	124.77	118.77
2	B	1290	NAP	C2A-N1A-C6A	3.46	124.82	118.77
3	C	1281	HD2	C12-C8-C9	3.56	108.90	102.28
2	D	1291	NAP	C2A-N1A-C6A	3.66	125.18	118.77
2	C	1280	NAP	O2N-PN-O1N	3.78	131.87	112.28
3	B	1291	HD2	C28-C27-N7	3.80	120.43	111.98
2	A	1290	NAP	C5N-C6N-N1N	4.01	126.57	120.40
2	A	1290	NAP	C2A-N1A-C6A	4.15	126.03	118.77
2	C	1280	NAP	C4B-O4B-C1B	4.57	114.64	109.77
2	D	1291	NAP	C5N-C6N-N1N	4.65	127.56	120.40
2	B	1290	NAP	O3X-P2B-O2X	5.60	130.19	107.61
2	A	1290	NAP	O3X-P2B-O2X	5.89	131.38	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1290	NAP	C5N-C6N-N1N	6.01	129.65	120.40
2	D	1291	NAP	O3X-P2B-O2X	6.24	132.78	107.61
2	C	1280	NAP	O3X-P2B-O2X	6.48	133.76	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1290	NAP	2	0
3	A	1291	HD2	2	0
3	B	1291	HD2	1	0
2	C	1280	NAP	1	0
3	C	1281	HD2	1	0
3	D	1292	HD2	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	263/292 (90%)	-0.13	11 (4%) 37 35	5, 21, 49, 69	0
1	B	264/292 (90%)	-0.32	4 (1%) 74 72	6, 18, 52, 68	0
1	C	254/292 (86%)	-0.34	3 (1%) 79 77	9, 17, 42, 74	0
1	D	262/292 (89%)	0.08	11 (4%) 37 35	10, 30, 58, 71	0
All	All	1043/1168 (89%)	-0.18	29 (2%) 53 51	5, 22, 52, 74	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	233	MET	6.9
1	A	263	TRP	5.4
1	A	282	THR	4.9
1	A	262	ARG	4.6
1	C	266	LEU	3.9
1	D	287	ASP	3.9
1	A	232	HIS	3.3
1	A	280	TYR	3.1
1	C	279	LEU	3.0
1	D	282	THR	2.9
1	D	283	SER	2.9
1	D	280	TYR	2.7
1	A	287	ASP	2.7
1	A	130	HIS	2.7
1	D	290	ILE	2.6
1	A	283	SER	2.5
1	B	232	HIS	2.4
1	D	80	GLU	2.3
1	A	284	TYR	2.3
1	D	28	ARG	2.2
1	A	266	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	30	GLU	2.1
1	C	232	HIS	2.1
1	D	69	GLU	2.1
1	B	280	TYR	2.1
1	A	260	SER	2.1
1	B	28	ARG	2.0
1	D	284	TYR	2.0
1	B	279	LEU	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. 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	HD2	B	1291	31/31	0.95	0.12	-0.32	12,15,39,43	0
3	HD2	D	1292	31/31	0.92	0.12	-0.33	21,28,41,45	0
3	HD2	C	1281	31/31	0.94	0.11	-0.40	10,16,36,40	0
3	HD2	A	1291	31/31	0.94	0.12	-0.42	15,21,42,44	0
2	NAP	C	1280	48/48	0.98	0.09	-0.50	7,12,16,21	0
2	NAP	D	1291	48/48	0.95	0.10	-0.73	15,21,31,33	0
2	NAP	B	1290	48/48	0.99	0.07	-1.06	5,10,14,22	0
2	NAP	A	1290	48/48	0.98	0.08	-1.13	5,14,19,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.