



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:36 AM GMT

PDB ID : 2B23  
Title : Human estrogen receptor alpha ligand-binding domain and a glucocorticoid receptor-interacting protein 1 NR box II peptide  
Authors : Rajan, S.S.; Hsieh, R.W.; Sharma, S.K.; Greene, G.L.  
Deposited on : 2005-09-16  
Resolution : 2.10 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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

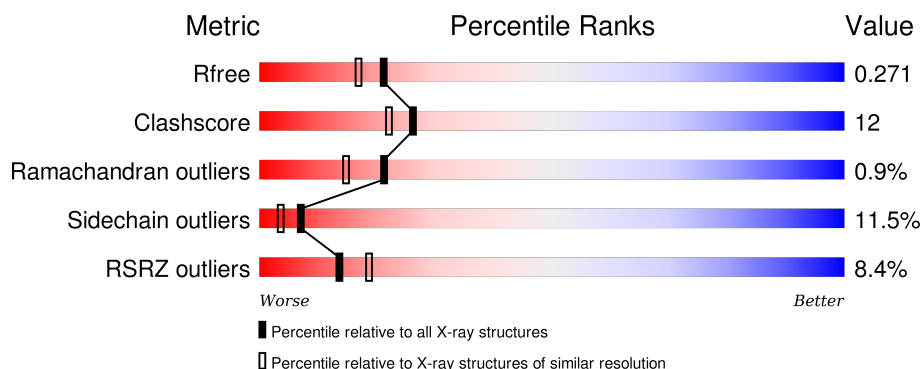
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	257	<div> <div>9%</div> <div>61%</div> <div>23%</div> <div>•</div> <div>11%</div> </div>
1	B	257	<div> <div>7%</div> <div>68%</div> <div>19%</div> <div>•</div> <div>9%</div> </div>
2	C	13	<div> <div>8%</div> <div>46%</div> <div>31%</div> <div>23%</div> </div>
2	D	13	<div> <div>31%</div> <div>38%</div> <div>31%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3936 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	3	0
			1853	1185	317	329	22			
1	B	233	Total	C	N	O	S	0	3	0
			1885	1206	321	334	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	CME	CYS	MODIFIED RESIDUE	UNP P03372
A	417	CME	CYS	MODIFIED RESIDUE	UNP P03372
A	530	CME	CYS	MODIFIED RESIDUE	UNP P03372
A	537	SER	TYR	ENGINEERED	UNP P03372
B	381	CME	CYS	MODIFIED RESIDUE	UNP P03372
B	417	CME	CYS	MODIFIED RESIDUE	UNP P03372
B	530	CME	CYS	MODIFIED RESIDUE	UNP P03372
B	537	SER	TYR	ENGINEERED	UNP P03372

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			89	57	19	13			
2	D	9	Total	C	N	O	0	0	0
			79	51	16	12			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	19	Total	O	0	0
			19	19		



LYS	
HIS	
K688	
H691	
H692	
L693	
L694	
H695	
D696	
SER	
SER	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.37Å 80.91Å 58.24Å 90.00° 109.68° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 26.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.10) 94.5 (26.93-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.214 , 0.272 0.216 , 0.271	Depositor DCC
$R_{free}$ test set	1338 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 26279 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3936	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CME

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	0.44	0/1866	0.59	0/2514
1	B	0.42	0/1891	0.57	0/2551
2	C	0.39	0/90	0.46	0/119
2	D	0.44	0/79	0.51	0/104
All	All	0.43	0/3926	0.58	0/5288

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	1853	0	1888	59	0
1	B	1885	0	1930	44	0
2	C	89	0	95	2	0
2	D	79	0	88	3	0
3	A	11	0	0	1	0
3	B	19	0	0	0	0
All	All	3936	0	4001	97	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 12.

All (97) 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:363:ARG:HH21	1:A:363:ARG:HG2	1.07	1.09
1:A:458:VAL:HG21	1:A:475:ILE:HD12	1.51	0.93
1:B:528:MET:CE	1:B:534:VAL:HG21	2.02	0.88
1:A:363:ARG:HG2	1:A:363:ARG:NH2	1.87	0.87
1:A:458:VAL:CG2	1:A:475:ILE:HD12	2.09	0.81
1:A:547:HIS:O	1:A:548:ARG:HB2	1.80	0.79
1:A:337:PHE:N	1:A:417:CME:HH	1.84	0.76
1:A:401:LYS:HD3	1:A:409:LEU:HD23	1.68	0.75
1:B:528:MET:HE2	1:B:534:VAL:HG21	1.68	0.75
1:A:368:VAL:HG22	3:A:17:HOH:O	1.85	0.74
1:A:363:ARG:CG	1:A:363:ARG:HH21	1.96	0.73
1:A:404:PHE:CE2	1:A:410:LEU:HD12	2.26	0.71
1:A:532:ASN:O	1:A:532:ASN:ND2	2.19	0.71
1:A:525:LEU:HD23	1:A:544:LEU:HD13	1.73	0.69
1:A:547:HIS:O	1:A:548:ARG:CB	2.40	0.69
1:B:528:MET:HE3	1:B:534:VAL:HG21	1.75	0.66
1:A:380:GLU:O	1:A:547:HIS:HE1	1.78	0.65
1:A:459:TYR:OH	1:B:510:ILE:HG12	1.97	0.65
1:A:312:ALA:O	1:A:316:VAL:HG12	1.97	0.65
1:A:520:LYS:O	1:A:524[A]:HIS:HD2	1.80	0.65
1:A:404:PHE:CD2	1:A:410:LEU:HD12	2.31	0.64
1:A:414:GLN:O	1:A:417:CME:HB3	1.97	0.63
1:B:533:VAL:HG13	1:B:534:VAL:HG13	1.80	0.63
1:A:459:TYR:C	1:A:461:PHE:H	2.02	0.63
1:B:529:LYS:HG3	1:B:530:CME:N	2.14	0.63
1:A:435:PHE:HE2	1:A:510:ILE:HG21	1.63	0.62
1:A:383:TRP:CD1	1:A:543:MET:HE3	2.34	0.62
1:A:343:MET:O	1:A:347:THR:HG23	1.99	0.62
1:B:403:LEU:HD12	1:B:409:LEU:HG	1.81	0.61
1:A:435:PHE:CE2	1:A:510:ILE:HG21	2.37	0.60
1:B:412:ARG:HD3	1:B:426:ASP:OD2	2.03	0.59
1:A:380:GLU:O	1:A:547:HIS:CE1	2.57	0.57
1:A:377:HIS:HE1	1:A:457:GLY:O	1.87	0.56
1:B:420:GLY:O	1:B:421:MET:HB3	2.05	0.56
1:A:342:MET:HG2	1:A:418:VAL:HG21	1.88	0.56
1:A:497:LEU:HD22	1:B:497:LEU:HD11	1.88	0.56
1:A:342:MET:HG2	1:A:418:VAL:CG2	2.37	0.55
1:B:455:ASN:O	1:B:458:VAL:HG12	2.07	0.54
1:B:528:MET:HE2	1:B:534:VAL:CG2	2.37	0.53
1:B:424:ILE:HA	1:B:427:MET:HE3	1.91	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLN:O	1:A:506:GLN:HG3	2.09	0.52
1:A:475:ILE:C	1:A:475:ILE:HD13	2.30	0.52
1:A:513[A]:HIS:CE1	1:B:459:TYR:CD2	2.98	0.52
1:A:458:VAL:HG13	1:A:459:TYR:HD1	1.74	0.51
1:B:403:LEU:HD12	1:B:409:LEU:CG	2.41	0.51
1:A:530:CME:C	1:A:532:ASN:H	2.23	0.51
1:B:418:VAL:HB	1:B:421:MET:HG2	1.92	0.50
1:A:475:ILE:O	1:A:475:ILE:HD13	2.12	0.50
1:A:380:GLU:OE1	2:C:688:LYS:HE2	2.12	0.50
1:B:424:ILE:HA	1:B:427:MET:CE	2.42	0.50
1:A:329:SER:C	1:A:331:TYR:H	2.14	0.49
1:A:424:ILE:HD11	1:A:524[A]:HIS:CD2	2.47	0.49
1:A:316:VAL:HG22	1:A:320:LEU:HD22	1.94	0.49
1:B:420:GLY:O	1:B:524:HIS:CD2	2.66	0.49
1:A:474:HIS:O	1:A:478:VAL:HG23	2.12	0.49
1:B:339:GLU:HB2	1:B:418:VAL:HG22	1.95	0.48
1:A:513[A]:HIS:CD2	1:B:459:TYR:HD2	2.31	0.48
1:B:372:LEU:HD12	2:D:691:HIS:ND1	2.29	0.48
1:A:458:VAL:O	1:A:461:PHE:HB2	2.14	0.47
1:A:458:VAL:HG23	1:A:475:ILE:HD12	1.93	0.47
1:A:337:PHE:O	1:A:417:CME:SG	2.72	0.47
1:A:392:VAL:HG13	1:A:432:SER:HA	1.96	0.47
1:A:376:VAL:HG13	2:C:690:LEU:HD23	1.96	0.47
1:B:362:LYS:HE2	2:D:694:LEU:O	2.14	0.47
1:B:412:ARG:HB3	1:B:429:LEU:CD2	2.45	0.47
1:A:536:LEU:HD22	1:A:540:LEU:HD13	1.96	0.47
1:A:383:TRP:CD1	1:A:543:MET:CE	2.97	0.47
1:B:332:ASP:OD2	1:B:334:THR:HB	2.15	0.47
1:B:308:LEU:N	1:B:308:LEU:HD12	2.31	0.46
1:A:520:LYS:O	1:A:524[A]:HIS:CD2	2.66	0.46
1:B:416:LYS:HB2	1:B:417:CME:HZ2	1.97	0.46
1:B:533:VAL:HG13	1:B:534:VAL:N	2.31	0.46
1:B:448:LEU:HD21	1:B:507:LEU:HB3	1.98	0.46
1:B:528:MET:HE2	1:B:528:MET:HB3	1.74	0.45
1:B:381[B]:CME:HZ3	1:B:457:GLY:HA2	1.99	0.45
1:A:513[A]:HIS:CE1	1:B:459:TYR:CE2	3.05	0.45
1:A:532:ASN:C	1:A:532:ASN:HD22	2.15	0.44
1:A:519:ASN:HD22	1:B:519:ASN:HD22	1.65	0.44
1:B:424:ILE:HD13	1:B:427:MET:CE	2.48	0.44
1:B:372:LEU:HD22	1:B:372:LEU:HA	1.88	0.44
1:B:481:LYS:HE3	1:B:481:LYS:HB3	1.75	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLU:HG3	1:A:418:VAL:HG13	2.00	0.44
1:A:530:CME:C	1:A:532:ASN:N	2.81	0.44
1:A:541:LEU:O	1:A:545:ASP:HB2	2.18	0.44
1:A:392:VAL:HG13	1:A:432:SER:CA	2.48	0.44
2:D:688:LYS:HE2	2:D:688:LYS:HB2	1.87	0.44
1:A:372:LEU:O	1:A:376:VAL:HG23	2.17	0.43
1:B:540:LEU:HA	1:B:540:LEU:HD12	1.82	0.43
1:B:529:LYS:HG3	1:B:530:CME:H	1.83	0.43
1:B:315:MET:SD	1:B:365:PRO:HG2	2.59	0.42
1:A:458:VAL:HG21	1:A:475:ILE:CD1	2.36	0.42
1:B:497:LEU:HD22	1:B:501[A]:HIS:CE1	2.55	0.42
1:B:354:LEU:HD21	1:B:543:MET:HG3	2.02	0.42
1:A:501:HIS:CG	1:B:487:ILE:HG13	2.55	0.41
1:B:486:LEU:HA	1:B:486:LEU:HD23	1.88	0.41
1:B:381[B]:CME:HZ2	1:B:515:ARG:HH12	1.85	0.41
1:B:498:GLN:HA	1:B:501[B]:HIS:CE1	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	223/257 (87%)	215 (96%)	6 (3%)	2 (1%)	21	15
1	B	228/257 (89%)	223 (98%)	3 (1%)	2 (1%)	21	15
2	C	8/13 (62%)	8 (100%)	0	0	100	100
2	D	7/13 (54%)	7 (100%)	0	0	100	100
All	All	466/540 (86%)	453 (97%)	9 (2%)	4 (1%)	21	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	421	MET
1	A	460	THR
1	A	306	LEU
1	B	420	GLY

### 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	205/229 (90%)	180 (88%)	25 (12%)	6	3
1	B	208/229 (91%)	188 (90%)	20 (10%)	10	6
2	C	10/13 (77%)	8 (80%)	2 (20%)	1	0
2	D	9/13 (69%)	7 (78%)	2 (22%)	1	0
All	All	432/484 (89%)	383 (89%)	49 (11%)	7	4

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	LEU
1	A	317	SER
1	A	320	LEU
1	A	327	LEU
1	A	330	GLU
1	A	345	LEU
1	A	346	LEU
1	A	349	LEU
1	A	363	ARG
1	A	368	VAL
1	A	378	LEU
1	A	409	LEU
1	A	411	ASP
1	A	424	ILE
1	A	460	THR
1	A	475	ILE
1	A	476	HIS
1	A	481	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	523	GLU
1	A	528	MET
1	A	532	ASN
1	A	533	VAL
1	A	540	LEU
1	A	541	LEU
1	A	545	ASP
1	B	321	ASP
1	B	346	LEU
1	B	349	LEU
1	B	354	LEU
1	B	372	LEU
1	B	421	MET
1	B	425	PHE
1	B	429	LEU
1	B	432	SER
1	B	439	ASN
1	B	440	LEU
1	B	460	THR
1	B	473	ASP
1	B	481	LYS
1	B	492	LYS
1	B	497	LEU
1	B	525	LEU
1	B	529	LYS
1	B	540	LEU
1	B	544	LEU
2	C	687	HIS
2	C	696	ASP
2	D	692	ARG
2	D	693	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	HIS
1	A	516	HIS
1	A	547	HIS
1	B	439	ASN
1	B	476	HIS
1	B	519	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

7 non-standard protein/DNA/RNA residues 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$
1	CME	A	381	1	8,9,10	0.60	0	6,9,11	1.38	1 (16%)
1	CME	A	417	1	8,9,10	0.71	0	6,9,11	1.23	0
1	CME	A	530	1	8,9,10	0.77	0	6,9,11	1.76	2 (33%)
1	CME	B	381[A]	-	8,9,10	0.68	0	6,9,11	1.36	0
1	CME	B	381[B]	-	8,9,10	0.76	0	6,9,11	1.54	0
1	CME	B	417	1	8,9,10	0.69	0	6,9,11	1.14	0
1	CME	B	530	1	8,9,10	0.73	0	6,9,11	1.44	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
1	CME	A	381	1	-	0/5/8/10	0/0/0/0
1	CME	A	417	1	-	0/5/8/10	0/0/0/0
1	CME	A	530	1	-	0/5/8/10	0/0/0/0
1	CME	B	381[A]	-	-	0/5/8/10	0/0/0/0
1	CME	B	381[B]	-	-	0/5/8/10	0/0/0/0
1	CME	B	417	1	-	0/5/8/10	0/0/0/0
1	CME	B	530	1	-	0/5/8/10	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	530	CME	CB-SG-SD	-2.85	98.39	103.95
1	A	381	CME	CB-SG-SD	-2.37	99.34	103.95
1	A	530	CME	O-C-CA	-2.20	119.76	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	417	CME	3	0
1	A	530	CME	2	0
1	B	381[B]	CME	2	0
1	B	417	CME	1	0
1	B	530	CME	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	226/257 (87%)	0.35	22 (9%) 10 14	17, 29, 53, 70	0
1	B	230/257 (89%)	0.34	17 (7%) 17 24	19, 31, 51, 72	0
2	C	10/13 (76%)	0.34	1 (10%) 9 13	29, 37, 54, 58	0
2	D	9/13 (69%)	0.57	0 100 100	30, 39, 46, 55	0
All	All	475/540 (87%)	0.35	40 (8%) 14 19	17, 30, 54, 72	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	533	VAL	6.2
1	A	533	VAL	4.5
1	A	461	PHE	3.9
1	B	420	GLY	3.8
1	B	534	VAL	3.6
2	C	687	HIS	3.5
1	A	305	SER	3.5
1	B	412	ARG	3.4
1	B	419	GLU	3.4
1	A	332	ASP	3.4
1	A	420	GLY	3.4
1	B	461	PHE	3.2
1	A	331	TYR	3.0
1	B	532	ASN	3.0
1	B	421	MET	2.8
1	A	534	VAL	2.8
1	A	452	ILE	2.7
1	B	459	TYR	2.6
1	B	511	LEU	2.6
1	A	451	ILE	2.6
1	B	373	HIS	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	535	PRO	2.5
1	A	460	THR	2.5
1	A	513[A]	HIS	2.5
1	A	340	ALA	2.4
1	B	413	ASN	2.4
1	A	548	ARG	2.4
1	A	419	GLU	2.3
1	A	528	MET	2.3
1	A	386	ILE	2.3
1	A	535	PRO	2.3
1	B	305	SER	2.2
1	A	473	ASP	2.2
1	A	448	LEU	2.2
1	A	338	SER	2.1
1	A	418	VAL	2.1
1	A	321	ASP	2.1
1	B	339	GLU	2.1
1	B	453	LEU	2.1
1	B	337	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	CME	A	530	10/11	0.91	0.18	-	45,51,71,76	0
1	CME	B	381[A]	10/11	0.94	0.14	-	21,27,48,50	6
1	CME	B	381[B]	10/11	0.94	0.14	-	21,27,47,48	6
1	CME	A	417	10/11	0.59	0.30	-	47,71,78,80	0
1	CME	A	381	10/11	0.92	0.12	-	16,24,55,55	0
1	CME	B	417	10/11	0.60	0.39	-	65,74,78,80	0
1	CME	B	530	10/11	0.93	0.22	-	45,50,72,73	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.