



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:02 AM GMT

PDB ID : 2FAI
Title : Human Estrogen Receptor Alpha Ligand-Binding Domain In Complex With
OBCP-2M 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 : 2005-12-07
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
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

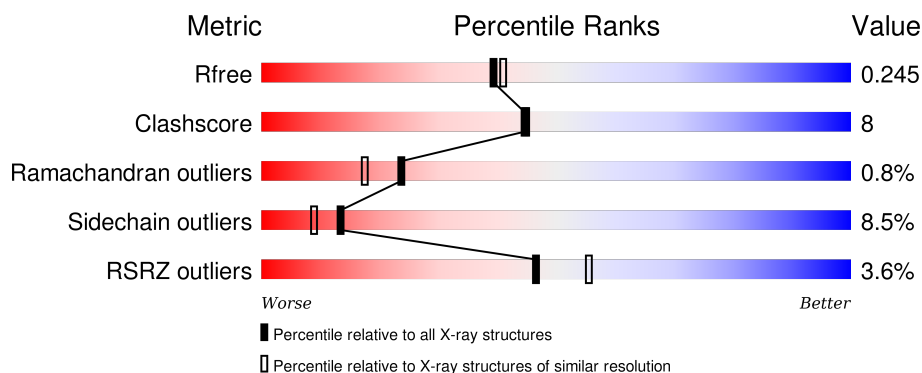
1 Overall quality at a glance

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 ≥ 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>4%</div> <div>72%</div> <div>16%</div> <div>8%</div> </div>
1	B	257	<div> <div>3%</div> <div>74%</div> <div>18%</div> <div>5%</div> </div>
2	C	13	<div> <div>8%</div> <div>54%</div> <div>15%</div> <div>8%</div> <div>23%</div> </div>
2	D	13	<div> <div>54%</div> <div>23%</div> <div>23%</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	459	A	101	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4142 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	236	Total	C	N	O	S	0	6	0
			1924	1228	329	343	24			
1	B	245	Total	C	N	O	S	0	2	0
			1974	1259	336	355	24			

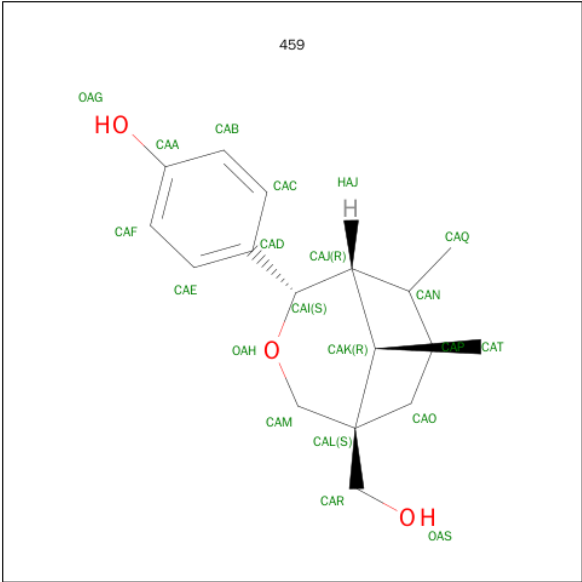
There are 8 discrepancies between the modelled and reference sequences:

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	10	Total	C	N	O	0	0	0
			89	57	19	13			

- Molecule 3 is 4-[(1S,2S,5S,9R)-5-(HYDROXYMETHYL)-8,9-DIMETHYL-3-OXABICYCLO[3.3.1]NON-7-EN-2-YL]PHENOL (three-letter code: 459) (formula: C₁₇H₂₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	17	3		
3	B	1	Total	C	O	0	1
			21	18	3		

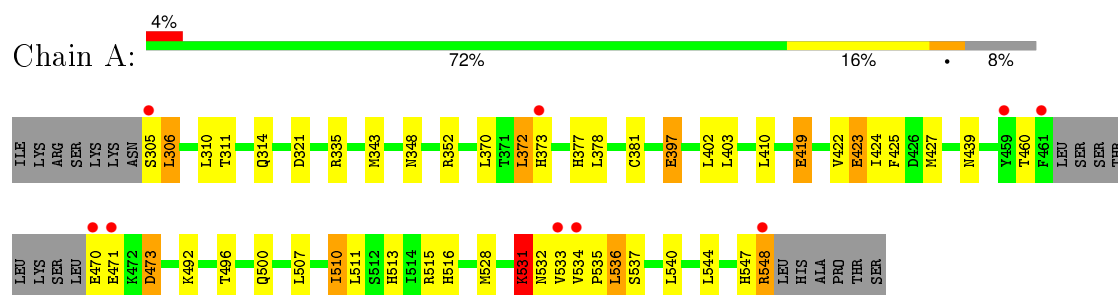
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	15	Total	O	0	0
			15	15		

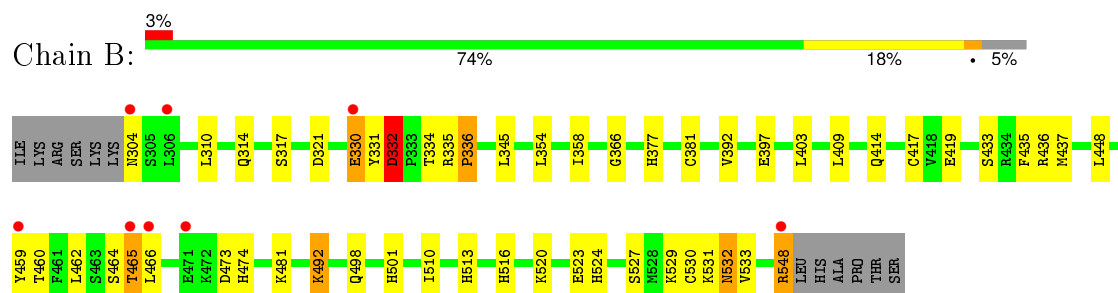
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Estrogen receptor



• Molecule 1: Estrogen receptor



• Molecule 2: Nuclear receptor coactivator 2



• Molecule 2: Nuclear receptor coactivator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.40 Å 81.81 Å 58.86 Å 90.00° 111.16° 90.00°	Depositor
Resolution (Å)	19.62 – 2.10 19.62 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.62-2.10) 99.0 (19.62-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.09 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.240 0.210 , 0.245	Depositor DCC
R_{free} test set	1455 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.6	EDS
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 28829 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4142	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 459, 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	0.37	0/1943	0.66	8/2620 (0.3%)
1	B	0.36	0/1976	0.67	9/2666 (0.3%)
2	C	0.31	0/90	0.86	2/119 (1.7%)
2	D	0.33	0/90	0.55	0/119
All	All	0.36	0/4099	0.67	19/5524 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	0	1
All	All	1	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	548	ARG	CB-CA-C	-13.32	83.76	110.40
1	A	423	GLU	CB-CA-C	13.20	136.80	110.40
1	A	492	LYS	CB-CA-C	-6.43	97.54	110.40
1	A	531	LYS	CB-CA-C	-6.42	97.55	110.40
1	B	332	ASP	CB-CA-C	-6.42	97.57	110.40
1	B	523	GLU	CB-CA-C	-6.37	97.66	110.40
1	B	492	LYS	CB-CA-C	-6.26	97.88	110.40
2	C	687	HIS	CB-CA-C	-6.16	98.08	110.40
1	B	397	GLU	CB-CA-C	5.94	122.28	110.40
1	A	419	GLU	CB-CA-C	5.92	122.24	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	GLU	CB-CA-C	5.87	122.15	110.40
1	A	532	ASN	CB-CA-C	5.71	121.83	110.40
1	A	471	GLU	CB-CA-C	5.71	121.82	110.40
1	B	419	GLU	CB-CA-C	5.64	121.69	110.40
1	B	473	ASP	CB-CA-C	5.45	121.30	110.40
1	B	304	ASN	CB-CA-C	5.33	121.07	110.40
1	A	470	GLU	CB-CA-C	5.30	121.01	110.40
1	A	473	ASP	CB-CA-C	5.28	120.97	110.40
2	C	696	ASP	CB-CA-C	5.20	120.79	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	423	GLU	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	335	ARG	Peptide

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	1924	0	1960	44	0
1	B	1974	0	2027	27	0
2	C	89	0	95	2	0
2	D	89	0	95	1	0
3	A	20	0	23	1	0
3	B	21	0	8	1	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
All	All	4142	0	4208	66	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 8.

All (66) 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:377:HIS:NE2	1:B:460:THR:HG23	1.87	0.88
1:A:381[B]:CME:HZ3	1:A:515:ARG:NH1	1.90	0.85
1:A:548:ARG:NH1	1:A:548:ARG:CB	2.44	0.81
1:A:548:ARG:CZ	1:A:548:ARG:HB2	2.10	0.81
1:B:403:LEU:HD13	1:B:409:LEU:HD13	1.62	0.80
1:A:397:GLU:CD	1:A:397:GLU:H	1.87	0.79
1:A:381[B]:CME:HZ3	1:A:515:ARG:HH11	1.49	0.77
1:A:548:ARG:NH1	1:A:548:ARG:HB2	2.01	0.74
1:A:548:ARG:HH11	1:A:548:ARG:HB3	1.59	0.68
1:A:348:ASN:ND2	1:A:352:ARG:HH21	1.93	0.66
1:A:548:ARG:CB	1:A:548:ARG:HH11	2.08	0.65
1:A:548:ARG:NH1	1:A:548:ARG:HB3	2.12	0.65
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.33	0.64
1:A:348:ASN:HD22	1:A:352:ARG:HH21	1.43	0.64
1:A:513[A]:HIS:CE1	1:B:459:TYR:CD1	2.85	0.64
1:A:311:THR:HG23	1:A:314:GLN:H	1.64	0.62
1:B:510:ILE:HA	1:B:513[A]:HIS:HD2	1.64	0.62
1:B:465:THR:O	1:B:466:LEU:HB2	1.97	0.62
1:B:527:SER:O	1:B:531:LYS:HD3	1.99	0.61
1:A:311:THR:CG2	1:A:314:GLN:H	2.13	0.60
1:A:377:HIS:NE2	1:A:460:THR:HG23	2.17	0.60
1:A:496:THR:O	1:A:500:GLN:HG3	2.01	0.59
1:A:381[B]:CME:HE2	1:B:516:HIS:CE1	2.37	0.59
1:B:530:CME:C	1:B:532:ASN:H	2.14	0.59
1:A:381[B]:CME:HE3	1:A:547:HIS:HE1	1.67	0.58
1:A:397:GLU:N	1:A:397:GLU:CD	2.55	0.58
1:A:403:LEU:HD23	1:A:403:LEU:O	2.05	0.56
1:A:548:ARG:CZ	1:A:548:ARG:CB	2.82	0.55
1:A:507:LEU:O	1:A:510:ILE:HG12	2.07	0.54
1:A:422:VAL:HG13	1:A:423:GLU:HG3	1.90	0.54
1:A:531:LYS:HB3	1:A:533:VAL:HG23	1.90	0.53
1:A:536:LEU:HD12	1:A:540:LEU:HD23	1.92	0.51
1:B:381[A]:CME:HZ2	1:B:460:THR:HG21	1.92	0.51
1:A:513[A]:HIS:CE1	1:B:459:TYR:HD1	2.27	0.51
1:A:381[B]:CME:HE3	1:A:547:HIS:CE1	2.46	0.50
1:A:311:THR:HG22	1:A:314:GLN:CG	2.41	0.50
2:C:687:HIS:CG	2:C:691:HIS:CD2	3.00	0.49
1:B:403:LEU:CD1	1:B:409:LEU:HD13	2.38	0.49
1:B:331:TYR:O	1:B:332:ASP:HB2	2.12	0.49
1:A:516:HIS:NE2	1:B:381[A]:CME:HE3	2.27	0.49
1:B:336:PRO:HA	1:B:417:CME:OH	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:SER:HA	1:B:436:ARG:HG2	1.96	0.48
2:D:691:HIS:O	2:D:695:GLN:HG3	2.13	0.48
1:A:534:VAL:HG22	1:A:535:PRO:HD2	1.96	0.47
1:B:414:GLN:O	1:B:417:CME:SG	2.73	0.46
1:B:377:HIS:CE1	1:B:460:THR:HG23	2.50	0.45
1:A:305:SER:O	1:A:306:LEU:HB2	2.17	0.45
1:B:530:CME:C	1:B:532:ASN:N	2.79	0.45
1:A:343:MET:CE	1:A:528:MET:HG3	2.46	0.45
1:A:343:MET:CE	3:A:101:459:HAR1	2.47	0.45
1:A:348:ASN:HD21	1:A:352:ARG:HE	1.66	0.44
1:A:513[A]:HIS:ND1	1:B:459:TYR:HD1	2.15	0.44
1:B:366:GLY:O	1:B:474:HIS:HE1	2.02	0.43
1:A:311:THR:HG22	1:A:314:GLN:CB	2.48	0.43
1:A:311:THR:HG22	1:A:314:GLN:HB2	2.01	0.43
1:A:348:ASN:ND2	1:A:352:ARG:HE	2.15	0.42
1:A:513[A]:HIS:CG	1:B:459:TYR:HD1	2.36	0.42
1:A:510:ILE:HG22	1:B:459:TYR:CE1	2.53	0.42
1:A:424:ILE:HA	1:A:427:MET:HE2	2.02	0.40
1:B:392:VAL:HG12	1:B:435:PHE:HD1	1.85	0.40
1:A:516:HIS:HE2	1:B:381[A]:CME:HE3	1.86	0.40
1:A:372:LEU:HD12	2:C:691:HIS:ND1	2.37	0.40
1:B:310:LEU:HD22	1:B:314:GLN:HB3	2.04	0.40
1:A:402:LEU:HD12	1:A:425:PHE:CD1	2.56	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	234/257 (91%)	231 (99%)	2 (1%)	1 (0%)	39	37
1	B	241/257 (94%)	232 (96%)	6 (2%)	3 (1%)	16	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	8/13 (62%)	8 (100%)	0	0	100	100
2	D	8/13 (62%)	8 (100%)	0	0	100	100
All	All	491/540 (91%)	479 (98%)	8 (2%)	4 (1%)	24	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	ASP
1	B	336	PRO
1	A	306	LEU
1	B	532	ASN

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	214/229 (93%)	193 (90%)	21 (10%)	10	6
1	B	219/229 (96%)	201 (92%)	18 (8%)	14	10
2	C	10/13 (77%)	10 (100%)	0	100	100
2	D	10/13 (77%)	9 (90%)	1 (10%)	9	6
All	All	453/484 (94%)	413 (91%)	40 (9%)	13	8

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	LEU
1	A	321	ASP
1	A	335	ARG
1	A	370	LEU
1	A	372	LEU
1	A	373[A]	HIS
1	A	373[B]	HIS
1	A	378	LEU

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Mol	Chain	Res	Type
1	A	397	GLU
1	A	410	LEU
1	A	419	GLU
1	A	439	ASN
1	A	473	ASP
1	A	510	ILE
1	A	511	LEU
1	A	531	LYS
1	A	536	LEU
1	A	537[A]	SER
1	A	537[B]	SER
1	A	544	LEU
1	A	548	ARG
1	B	317	SER
1	B	321	ASP
1	B	330	GLU
1	B	334	THR
1	B	345	LEU
1	B	354	LEU
1	B	358	ILE
1	B	437	MET
1	B	448	LEU
1	B	462	LEU
1	B	464	SER
1	B	465	THR
1	B	481	LYS
1	B	492	LYS
1	B	520	LYS
1	B	529	LYS
1	B	533	VAL
1	B	548	ARG
2	D	690	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	ASN
1	A	413	ASN
1	A	439	ASN
1	B	455	ASN
1	B	499	GLN
1	B	502	GLN

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Mol	Chain	Res	Type
2	C	687	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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[A]	-	8,9,10	0.79	0	6,9,11	1.92	1 (16%)
1	CME	A	381[B]	-	8,9,10	0.74	0	6,9,11	1.99	1 (16%)
1	CME	A	417	1	8,9,10	0.68	0	6,9,11	1.96	1 (16%)
1	CME	A	530	1	8,9,10	0.73	0	6,9,11	1.81	1 (16%)
1	CME	B	381[A]	-	8,9,10	0.72	0	6,9,11	2.15	1 (16%)
1	CME	B	381[B]	-	8,9,10	0.73	0	6,9,11	2.57	1 (16%)
1	CME	B	417	1	8,9,10	1.15	1 (12%)	6,9,11	2.12	3 (50%)
1	CME	B	530	1	8,9,10	0.69	0	6,9,11	1.84	1 (16%)

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[A]	-	-	0/5/8/10	0/0/0/0
1	CME	A	381[B]	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	417	CME	OH-CZ	2.11	1.53	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	417	CME	OH-CZ-CE	-2.37	100.45	110.83
1	B	417	CME	CZ-CE-SD	-2.01	108.25	113.16
1	A	530	CME	CB-SG-SD	3.38	110.54	103.95
1	A	381[A]	CME	CB-SG-SD	3.58	110.92	103.95
1	B	530	CME	CB-SG-SD	3.58	110.94	103.95
1	B	417	CME	CB-SG-SD	3.74	111.23	103.95
1	A	381[B]	CME	CB-SG-SD	3.81	111.37	103.95
1	A	417	CME	CB-SG-SD	4.06	111.86	103.95
1	B	381[A]	CME	CB-SG-SD	4.74	113.18	103.95
1	B	381[B]	CME	CB-SG-SD	5.74	115.13	103.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	381[B]	CME	5	0
1	B	381[A]	CME	3	0
1	B	417	CME	2	0
1	B	530	CME	2	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 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	459	A	101	-	21,22,22	1.98	3 (14%)	25,33,33	2.93	7 (28%)
3	459	B	201[A]	-	21,22,22	1.97	3 (14%)	25,33,33	2.57	6 (24%)
3	459	B	201[B]	-	21,22,22	1.97	3 (14%)	25,33,33	2.57	7 (28%)

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	459	A	101	-	1/1/5/5	0/7/37/37	0/1/3/3
3	459	B	201[A]	-	-	0/7/37/37	0/1/3/3
3	459	B	201[B]	-	-	0/7/37/37	0/1/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201[B]	459	CAP-CAN	-5.91	1.40	1.53
3	B	201[A]	459	CAP-CAN	-5.91	1.40	1.53
3	A	101	459	CAP-CAN	-5.71	1.40	1.53
3	B	201[B]	459	CAO-CAP	-5.68	1.40	1.53
3	B	201[A]	459	CAO-CAP	-5.68	1.40	1.53
3	A	101	459	CAO-CAP	-5.45	1.41	1.53
3	B	201[B]	459	CAD-CAI	2.16	1.54	1.51
3	B	201[A]	459	CAD-CAI	2.16	1.54	1.51
3	A	101	459	CAD-CAI	2.65	1.55	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	101	459	OAH-CAM-CAL	-6.60	105.62	111.07
3	A	101	459	CAN-CAJ-CAK	-4.25	103.69	109.65
3	B	201[B]	459	OAH-CAM-CAL	-3.64	108.06	111.07
3	B	201[A]	459	OAH-CAM-CAL	-3.64	108.06	111.07
3	B	201[B]	459	CAN-CAJ-CAK	-3.37	104.93	109.65
3	B	201[A]	459	CAN-CAJ-CAK	-3.37	104.93	109.65
3	B	201[B]	459	CAT-CAK-CAL	-2.19	111.60	114.40
3	A	101	459	CAT-CAK-CAL	-2.15	111.65	114.40
3	A	101	459	CAP-CAN-CAJ	3.29	116.84	110.37
3	A	101	459	CAQ-CAN-CAJ	3.41	120.08	114.18
3	B	201[B]	459	CAQ-CAN-CAJ	3.51	120.26	114.18
3	B	201[A]	459	CAQ-CAN-CAJ	3.51	120.26	114.18
3	B	201[B]	459	CAP-CAN-CAJ	3.95	118.14	110.37
3	B	201[A]	459	CAP-CAN-CAJ	3.95	118.14	110.37
3	B	201[B]	459	CAQ-CAN-CAP	6.26	121.59	110.84
3	B	201[A]	459	CAQ-CAN-CAP	6.26	121.59	110.84
3	A	101	459	CAQ-CAN-CAP	7.11	123.06	110.84
3	B	201[B]	459	CAO-CAP-CAN	7.75	127.12	112.17
3	B	201[A]	459	CAO-CAP-CAN	7.75	127.12	112.17
3	A	101	459	CAO-CAP-CAN	7.83	127.28	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	101	459	CAN

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	101	459	1	0
3	B	201[B]	459	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	233/257 (90%)	0.12	9 (3%) 43 52	15, 40, 58, 73	0
1	B	242/257 (94%)	0.12	8 (3%) 50 59	22, 39, 56, 72	0
2	C	10/13 (76%)	0.90	1 (10%) 9 13	43, 48, 60, 61	0
2	D	10/13 (76%)	0.04	0 100 100	40, 44, 56, 62	0
All	All	495/540 (91%)	0.14	18 (3%) 46 55	15, 40, 58, 73	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	SER	6.7
1	B	304	ASN	4.7
1	B	466	LEU	4.7
2	C	687	HIS	4.6
1	A	471	GLU	4.2
1	B	471	GLU	4.2
1	A	470	GLU	4.1
1	B	548	ARG	3.7
1	B	459	TYR	3.2
1	A	548	ARG	3.1
1	A	534	VAL	3.1
1	B	465	THR	2.8
1	B	330	GLU	2.8
1	A	459	TYR	2.8
1	A	533	VAL	2.7
1	A	373[A]	HIS	2.6
1	B	306	LEU	2.4
1	A	461	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(Å ²)	Q<0.9
1	CME	A	530	10/11	0.90	0.18	-	44,51,60,61	4
1	CME	A	417	10/11	0.84	0.19	-	31,41,44,48	5
1	CME	A	381[A]	10/11	0.94	0.15	-	33,35,56,58	6
1	CME	B	417	10/11	0.92	0.18	-	33,48,50,51	5
1	CME	B	381[B]	10/11	0.87	0.20	-	26,32,56,61	6
1	CME	A	381[B]	10/11	0.94	0.15	-	32,35,44,47	6
1	CME	B	530	10/11	0.92	0.14	-	50,52,59,61	4
1	CME	B	381[A]	10/11	0.87	0.20	-	28,37,62,66	6

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	459	B	201[B]	20/20	0.91	0.17	1.79	27,42,58,61	1
3	459	B	201[A]	20/20	0.91	0.17	1.79	20,38,53,61	1
3	459	A	101	20/20	0.89	0.15	1.09	32,37,56,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.