



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:39 AM UTC

PDB ID : 2B23 / pdb_00002b23
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

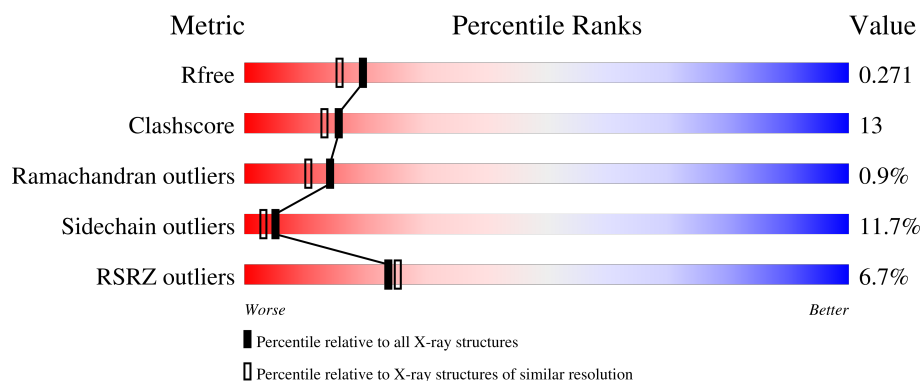
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	B	257	
2	C	13	
2	D	13	

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 mutation	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 mutation	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			

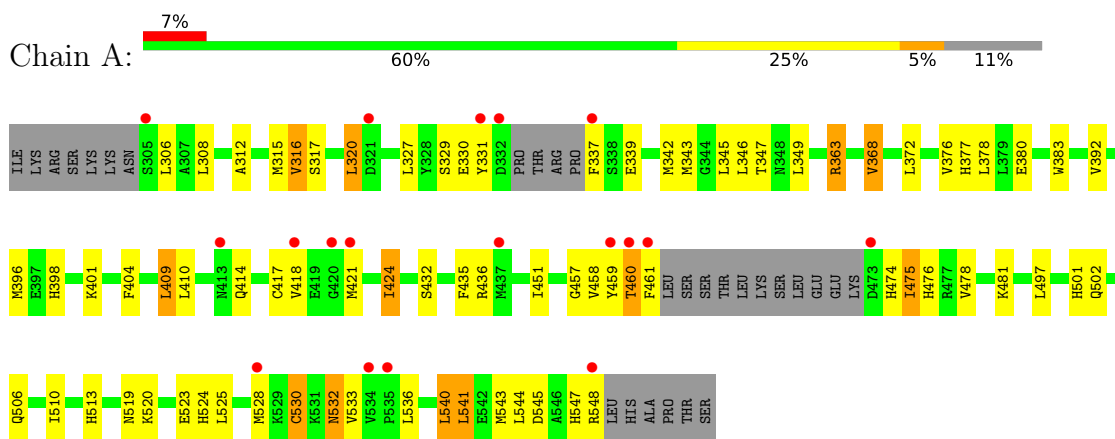
- Molecule 3 is water.

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

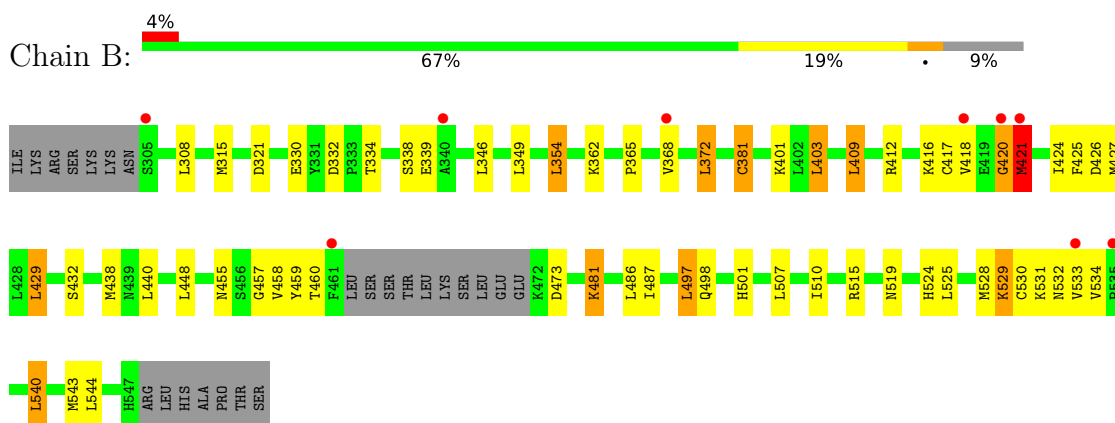
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Estrogen receptor



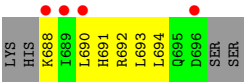
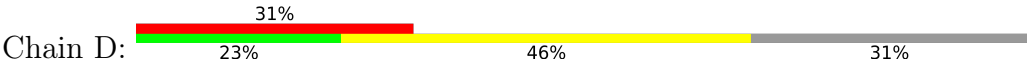
- Molecule 1: Estrogen receptor



- 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	54.37Å 80.91Å 58.24Å 90.00° 109.68° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.10) 94.5 (30.00-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005, XTALVIEW	Depositor
R, R_{free}	0.214 , 0.272 0.216 , 0.271	Depositor DCC
R_{free} test set	1338 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3936	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.62	1/1866 (0.1%)	0.83	2/2514 (0.1%)
1	B	0.56	0/1891	0.82	1/2551 (0.0%)
2	C	0.47	0/90	0.70	0/119
2	D	0.53	0/79	0.82	0/104
All	All	0.59	1/3926 (0.0%)	0.83	3/5288 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	ILE	CA-CB	5.82	1.61	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	LYS	N-CA-C	5.21	117.10	109.24
1	A	398	HIS	CA-C-N	5.06	125.06	119.90
1	A	398	HIS	C-N-CA	5.06	125.06	119.90

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	1853	0	1888	65	0
1	B	1885	0	1930	47	0
2	C	89	0	95	2	0
2	D	79	0	88	4	0
3	A	11	0	0	1	0
3	B	19	0	0	0	0
All	All	3936	0	4001	106	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 13.

All (106) 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:B:528:MET:HE3	1:B:534:VAL:HG21	1.07	1.06
1:B:528:MET:HE3	1:B:534:VAL:CG2	1.95	0.96
1:A:458:VAL:HG21	1:A:475:ILE:HD12	1.51	0.93
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:B:528:MET:CE	1:B:534:VAL:HG21	2.02	0.79
1:A:547:HIS:O	1:A:548:ARG:HB2	1.80	0.79
1:A:337:PHE:N	1:A:417:CME:HH	1.83	0.77
1:A:401:LYS:HD3	1:A:409:LEU:HD23	1.68	0.75
1:A:368:VAL:HG22	3:A:17:HOH:O	1.85	0.74
1:A:363:ARG:HH21	1:A:363:ARG:CG	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:383:TRP:CD1	1:A:543:MET:HE3	2.27	0.70
1:A:525:LEU:HD23	1:A:544:LEU:HD13	1.73	0.69
1:B:424:ILE:HA	1:B:427:MET:HE3	1.73	0.69
1:A:547:HIS:O	1:A:548:ARG:CB	2.40	0.69
1:A:459:TYR:C	1:A:461:PHE:H	2.02	0.67
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:475:ILE:C	1:A:475:ILE:HD13	2.30	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:A:329:SER:C	1:A:331:TYR:H	2.14	0.54
1:A:502:GLN:O	1:A:506:GLN:HG3	2.09	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:532:ASN:HD22	1:A:532:ASN:C	2.15	0.50
1:A:380:GLU:OE1	2:C:688:LYS:HE2	2.12	0.50
1:A:475:ILE:HD13	1:A:475:ILE:O	2.12	0.50
1:A:459:TYR:C	1:A:461:PHE:N	2.70	0.50
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:A:343:MET:SD	1:A:421:MET:HE1	2.53	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:424:ILE:HA	1:B:427:MET:CE	2.42	0.48
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:337:PHE:O	1:A:417:CME:SG	2.72	0.47
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: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:A:536:LEU:HD22	1:A:540:LEU:HD13	1.96	0.47
1:B:412:ARG:HB3	1:B:429:LEU:CD2	2.45	0.47
1:B:332:ASP:OD2	1:B:334:THR:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:TRP:CD1	1:A:543:MET:CE	2.97	0.46
1:B:308:LEU:HD12	1:B:308:LEU:N	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: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:519:ASN:HD22	1:B:519:ASN:HD22	1.65	0.44
1:B:372:LEU:HD22	1:B:372:LEU:HA	1.88	0.44
1:B:424:ILE:HD13	1:B:427:MET:CE	2.48	0.44
1:B:481:LYS:HE3	1:B:481:LYS:HB3	1.75	0.44
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:HB2	2:D:688:LYS:HE2	1.87	0.44
1:A:372:LEU:O	1:A:376:VAL:HG23	2.17	0.43
1:B:540:LEU:HD12	1:B:540:LEU:HA	1.82	0.43
1:B:529:LYS:HG3	1:B:530:CME:H	1.83	0.43
1:A:329:SER:C	1:A:331:TYR:N	2.77	0.43
1:B:424:ILE:HD13	1:B:427:MET:HE1	2.01	0.43
1:B:418:VAL:HB	1:B:421:MET:HE2	2.01	0.43
1:B:438:MET:HE2	1:B:438:MET:HB3	1.86	0.43
1:A:396:MET:HE3	1:A:436:ARG:HA	2.01	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:531:LYS:O	1:B:532:ASN:C	2.63	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:543:MET:HE1	2:D:690:LEU:HD22	2.02	0.41
1:B:486:LEU:HD23	1:B:486:LEU:HA	1.88	0.41
1:A:315:MET:HE2	1:A:315:MET:HB2	1.97	0.41
1:B:381[B]:CME:HZ2	1:B:515:ARG:HH12	1.85	0.41
1:A:532:ASN:ND2	1:A:532:ASN:C	2.78	0.40
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%)	14	10
1	B	228/257 (89%)	223 (98%)	3 (1%)	2 (1%)	14	10
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%)	14	10

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 [i](#)

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%)	181 (88%)	24 (12%)	5	3
1	B	208/229 (91%)	185 (89%)	23 (11%)	6	3
2	C	10/13 (77%)	9 (90%)	1 (10%)	7	5
2	D	9/13 (69%)	7 (78%)	2 (22%)	1	0
All	All	432/484 (89%)	382 (88%)	50 (12%)	5	3

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

Mol	Chain	Res	Type
1	A	308	LEU
1	A	316	VAL
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	424	ILE
1	A	460	THR
1	A	475	ILE
1	A	476	HIS
1	A	481	LYS
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	B	321	ASP
1	B	330	GLU
1	B	338	SER
1	B	346	LEU
1	B	349	LEU
1	B	354	LEU
1	B	368	VAL
1	B	372	LEU
1	B	403	LEU
1	B	409	LEU
1	B	421	MET
1	B	425	PHE
1	B	429	LEU
1	B	432	SER
1	B	440	LEU
1	B	460	THR
1	B	473	ASP
1	B	481	LYS

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Mol	Chain	Res	Type
1	B	497	LEU
1	B	525	LEU
1	B	529	LYS
1	B	540	LEU
1	B	544	LEU
2	C	696	ASP
2	D	692	ARG
2	D	693	LEU

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

Mol	Chain	Res	Type
1	A	359	ASN
1	A	377	HIS
1	A	516	HIS
1	A	547	HIS
1	B	439	ASN
1	B	519	ASN
1	B	524	HIS

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	B	381[B]	-	8,9,10	0.87	0	6,9,11	1.27	1 (16%)
1	CME	A	417	1	8,9,10	0.81	0	6,9,11	1.05	0
1	CME	A	381	1	8,9,10	0.69	0	6,9,11	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	B	381[A]	-	8,9,10	0.78	0	6,9,11	1.13	1 (16%)
1	CME	B	530	1	8,9,10	0.83	0	6,9,11	1.11	0
1	CME	A	530	1	8,9,10	0.86	0	6,9,11	1.33	1 (16%)
1	CME	B	417	1	8,9,10	0.79	0	6,9,11	0.88	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	B	381[B]	-	-	1/5/8/10	-
1	CME	A	417	1	-	3/5/8/10	-
1	CME	A	381	1	-	1/5/8/10	-
1	CME	B	381[A]	-	-	2/5/8/10	-
1	CME	B	530	1	-	1/5/8/10	-
1	CME	A	530	1	-	2/5/8/10	-
1	CME	B	417	1	-	2/5/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	381[A]	CME	CE-SD-SG	2.24	113.31	103.46
1	B	381[B]	CME	CE-SD-SG	2.20	113.11	103.46
1	A	530	CME	CB-SG-SD	-2.11	98.39	103.86

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	417	CME	N-CA-CB-SG
1	A	417	CME	CE-SD-SG-CB
1	A	417	CME	SD-CE-CZ-OH
1	A	530	CME	CZ-CE-SD-SG
1	B	417	CME	CA-CB-SG-SD
1	B	417	CME	CE-SD-SG-CB
1	B	381[A]	CME	CE-SD-SG-CB
1	B	381[B]	CME	CE-SD-SG-CB
1	A	530	CME	CE-SD-SG-CB

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Mol	Chain	Res	Type	Atoms
1	A	381	CME	SD-CE-CZ-OH
1	B	381[A]	CME	CZ-CE-SD-SG
1	B	530	CME	CZ-CE-SD-SG

There are no ring outliers.

5 monomers are involved in 10 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	226/257 (87%)	0.40	18 (7%) 18 19	13, 29, 53, 70	3 (1%)
1	B	230/257 (89%)	0.43	9 (3%) 43 45	15, 31, 51, 72	2 (0%)
2	C	10/13 (76%)	0.99	1 (10%) 12 13	29, 37, 54, 58	0
2	D	9/13 (69%)	1.92	4 (44%) 0 1	30, 39, 46, 55	0
All	All	475/540 (87%)	0.46	32 (6%) 24 25	13, 30, 54, 72	5 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	418	VAL	4.1
1	B	421	MET	3.9
1	A	331	TYR	3.6
1	A	305	SER	3.6
1	A	420	GLY	3.4
1	B	420	GLY	3.3
1	B	533	VAL	3.3
1	A	332	ASP	3.3
1	A	337	PHE	3.1
1	B	305	SER	3.1
2	D	689	ILE	3.0
2	C	687	HIS	2.9
1	A	460	THR	2.9
1	A	528	MET	2.8
1	B	535	PRO	2.8
2	D	696	ASP	2.7
1	A	534	VAL	2.7
1	A	461	PHE	2.6
1	A	459	TYR	2.6
1	B	368	VAL	2.6
1	A	548	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	340	ALA	2.5
1	A	421	MET	2.4
1	B	461	PHE	2.4
1	A	413	ASN	2.3
1	A	437	MET	2.3
1	A	418	VAL	2.2
1	A	473	ASP	2.2
1	A	321	ASP	2.2
1	A	535	PRO	2.1
2	D	688	LYS	2.1
2	D	690	LEU	2.1

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. 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(Å ²)	Q<0.9
1	CME	A	417	10/11	0.72	0.18	47,71,78,80	0
1	CME	B	417	10/11	0.75	0.15	65,74,78,80	0
1	CME	B	530	10/11	0.84	0.13	45,50,72,73	0
1	CME	A	530	10/11	0.86	0.12	45,51,71,76	0
1	CME	A	381	10/11	0.87	0.12	16,24,55,55	0
1	CME	B	381[A]	10/11	0.90	0.11	21,27,48,50	6
1	CME	B	381[B]	10/11	0.90	0.11	21,27,47,48	6

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.