



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:33 PM GMT

PDB ID : 1XQC  
Title : X-ray structure of ERalpha LBD bound to a tetrahydroisoquinoline SERM ligand at 2.05Å resolution  
Authors : Renaud, J.; Bischoff, S.F.; Buhl, T.; Floersheim, P.; Fournier, B.; Geiser, M.; Halleux, C.; Kallen, J.; Keller, H.J.; Ramage, P.  
Deposited on : 2004-10-12  
Resolution : 2.05 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 (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

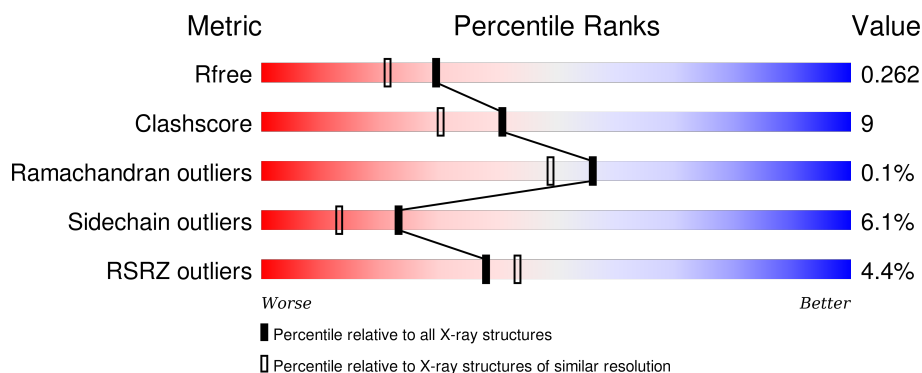
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	254	<div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	254	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>15%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	254	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	254	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>17%</div> <div>•</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7618 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.

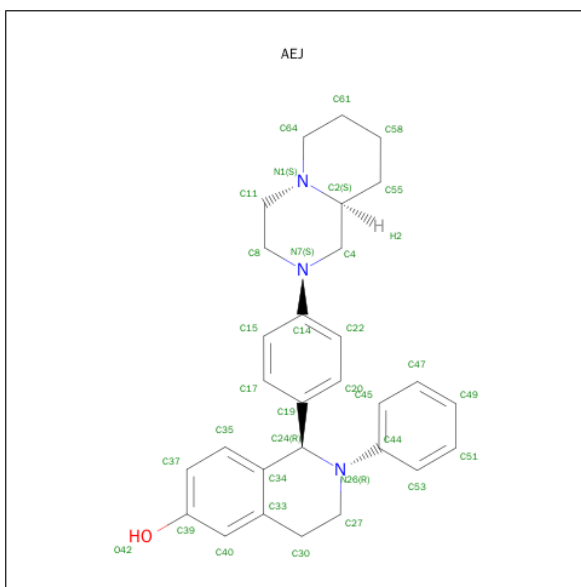
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1791	1148	306	321	16			
1	B	221	Total	C	N	O	S	0	0	0
			1765	1131	303	316	15			
1	C	224	Total	C	N	O	S	0	0	0
			1791	1148	306	321	16			
1	D	221	Total	C	N	O	S	0	0	0
			1765	1131	303	316	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	MET	-	INITIATING METHIONINE	UNP P03372
A	381	SER	CYS	ENGINEERED	UNP P03372
A	417	SER	CYS	ENGINEERED	UNP P03372
A	530	SER	CYS	ENGINEERED	UNP P03372
B	300	MET	-	INITIATING METHIONINE	UNP P03372
B	381	SER	CYS	ENGINEERED	UNP P03372
B	417	SER	CYS	ENGINEERED	UNP P03372
B	530	SER	CYS	ENGINEERED	UNP P03372
C	300	MET	-	INITIATING METHIONINE	UNP P03372
C	381	SER	CYS	ENGINEERED	UNP P03372
C	417	SER	CYS	ENGINEERED	UNP P03372
C	530	SER	CYS	ENGINEERED	UNP P03372
D	300	MET	-	INITIATING METHIONINE	UNP P03372
D	381	SER	CYS	ENGINEERED	UNP P03372
D	417	SER	CYS	ENGINEERED	UNP P03372
D	530	SER	CYS	ENGINEERED	UNP P03372

- Molecule 2 is (1S)-1-{4-[(9AR)-OCTAHYDRO-2H-PYRIDO[1,2-A]PYRAZIN-2-YL]PHE NYL}-2-PHENYL-1,2,3,4-TETRAHYDROISOQUINOLIN-6-OL (three-letter code: AEJ) (formula: C<sub>29</sub>H<sub>33</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	29	3	1		
2	B	1	Total	C	N	O	0	0
			33	29	3	1		
2	C	1	Total	C	N	O	0	0
			33	29	3	1		
2	D	1	Total	C	N	O	0	0
			33	29	3	1		

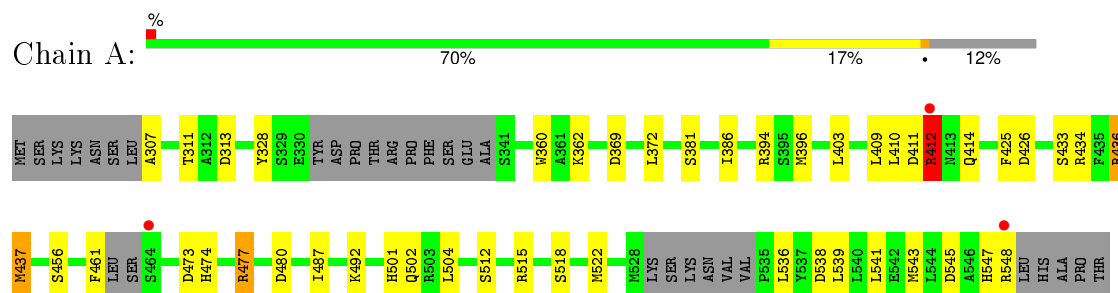
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	97	Total	O	0	0
			97	97		
3	B	87	Total	O	0	0
			87	87		
3	C	88	Total	O	0	0
			88	88		
3	D	102	Total	O	0	0
			102	102		

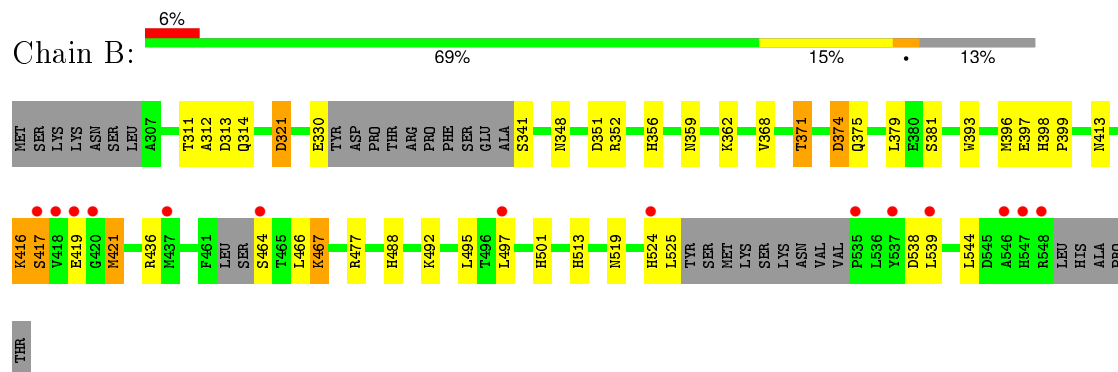
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

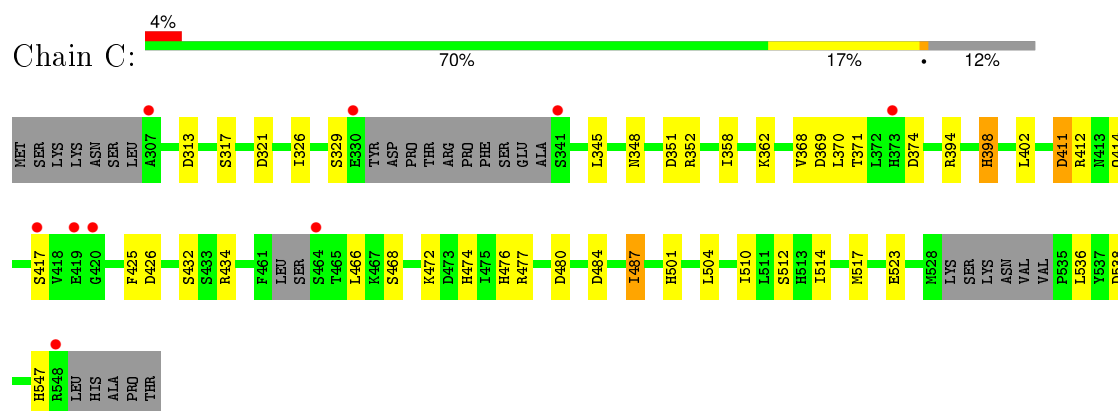
- Molecule 1: Estrogen receptor



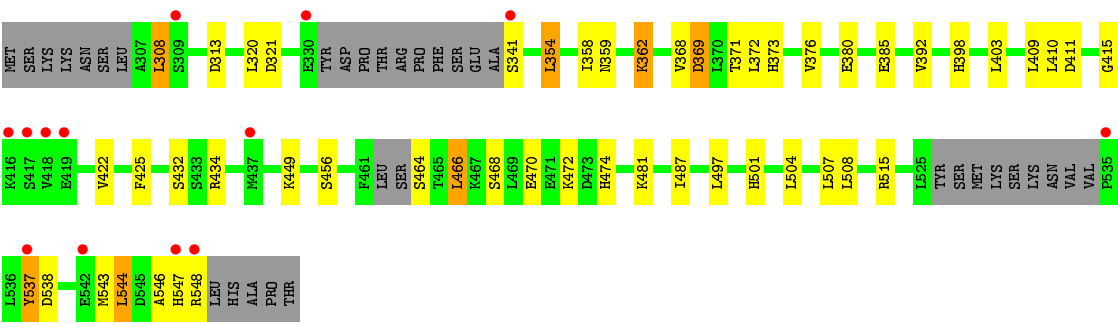
- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.11Å 156.57Å 58.96Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05 9.96 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.3 (10.00-2.05) 93.7 (9.96-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.211 , 0.254 0.223 , 0.262	Depositor DCC
$R_{free}$ test set	2992 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.148 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 58967 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AEJ

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	0.78	1/1821 (0.1%)	0.90	6/2454 (0.2%)
1	B	0.75	0/1794	0.87	5/2418 (0.2%)
1	C	0.73	0/1821	0.87	11/2454 (0.4%)
1	D	0.78	0/1794	0.90	5/2418 (0.2%)
All	All	0.76	1/7230 (0.0%)	0.88	27/9744 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	MET	CG-SD	5.52	1.95	1.81

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	313	ASP	CB-CG-OD2	9.07	126.47	118.30
1	B	351	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	480	ASP	CB-CG-OD2	6.82	124.44	118.30
1	C	321	ASP	CB-CG-OD2	6.81	124.43	118.30
1	C	394	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	538	ASP	CB-CG-OD2	6.50	124.15	118.30
1	C	480	ASP	CB-CG-OD2	6.39	124.06	118.30
1	C	374	ASP	CB-CG-OD2	6.25	123.93	118.30
1	C	313	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	394	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	D	538	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	426	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	484	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	411	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	394	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	D	369	ASP	CB-CG-OD2	5.56	123.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	411	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	321	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	538	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	538	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	473	ASP	CB-CG-OD2	5.27	123.05	118.30
1	C	351	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	313	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	321	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	412	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	374	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	426	ASP	CB-CG-OD2	5.01	122.81	118.30

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	1791	0	1840	34	1
1	B	1765	0	1817	32	1
1	C	1791	0	1840	30	0
1	D	1765	0	1817	39	0
2	A	33	0	33	1	0
2	B	33	0	33	0	0
2	C	33	0	33	0	0
2	D	33	0	33	1	0
3	A	97	0	0	8	0
3	B	87	0	0	12	0
3	C	88	0	0	8	0
3	D	102	0	0	7	0
All	All	7618	0	7446	126	1

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 9.

All (126) 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)
3:A:1039:HOH:O	1:B:513:HIS:HD2	1.56	0.88
1:D:398:HIS:CD2	3:D:4056:HOH:O	2.26	0.88
1:A:396:MET:O	1:A:436:ARG:NH1	2.11	0.84
1:D:422:VAL:O	3:D:4077:HOH:O	2.00	0.80
1:B:311:THR:HG23	1:B:314:GLN:H	1.48	0.78
1:A:412:ARG:HG3	1:A:412:ARG:HH11	1.49	0.78
1:B:311:THR:HG21	3:B:2038:HOH:O	1.83	0.77
1:D:466:LEU:HD22	1:D:466:LEU:O	1.85	0.77
1:B:419:GLU:HG2	1:C:368:VAL:HG13	1.67	0.75
1:B:371:THR:HB	3:B:2082:HOH:O	1.86	0.75
1:C:369:ASP:HB2	1:C:474:HIS:HE1	1.51	0.75
1:A:362:LYS:HG3	1:A:547:HIS:ND1	2.03	0.73
1:C:348:ASN:HD22	1:C:352:ARG:HH21	1.38	0.70
1:C:468:SER:HB3	3:C:3071:HOH:O	1.92	0.69
1:D:497:LEU:O	1:D:501:HIS:ND1	2.25	0.69
1:D:398:HIS:NE2	3:D:4056:HOH:O	2.26	0.69
1:B:371:THR:CG2	3:B:2082:HOH:O	2.43	0.67
1:D:359:ASN:HB3	3:D:4047:HOH:O	1.92	0.67
1:C:468:SER:CB	3:C:3071:HOH:O	2.43	0.66
1:B:374:ASP:CG	3:B:2082:HOH:O	2.34	0.65
1:A:545:ASP:O	1:A:548:ARG:HB2	1.97	0.65
1:D:398:HIS:CE1	3:D:4056:HOH:O	2.50	0.64
1:B:321:ASP:HB3	3:B:2085:HOH:O	1.98	0.64
1:D:354:LEU:O	1:D:358:ILE:HD12	1.98	0.63
1:C:501:HIS:HB2	3:C:3042:HOH:O	1.99	0.62
1:C:487:ILE:HD11	1:C:504:LEU:HD22	1.80	0.62
1:C:369:ASP:CB	1:C:474:HIS:HE1	2.13	0.61
1:D:415:GLY:HA3	1:D:425:PHE:CE2	2.34	0.61
1:D:362:LYS:CE	1:D:368:VAL:HG12	2.30	0.61
1:B:371:THR:CB	3:B:2082:HOH:O	2.47	0.60
1:D:456:SER:HA	1:D:515:ARG:NH2	2.16	0.59
1:C:402:LEU:HD12	1:C:425:PHE:CE2	2.38	0.59
1:B:525:LEU:O	3:B:2064:HOH:O	2.16	0.59
1:D:398:HIS:CG	3:D:4056:HOH:O	2.50	0.58
1:B:416:LYS:O	3:B:2053:HOH:O	2.17	0.58
1:D:409:LEU:C	1:D:410:LEU:HD23	2.24	0.58
1:A:403:LEU:CD1	1:A:409:LEU:HD13	2.34	0.57
1:A:539:LEU:O	1:A:543:MET:HG3	2.05	0.57
1:A:536:LEU:HD21	2:A:1001:AEJ:H581	1.86	0.56
1:A:434:ARG:HA	1:A:437:MET:HG2	1.87	0.56
1:C:362:LYS:HG3	1:C:547:HIS:ND1	2.21	0.56
1:B:413:ASN:O	1:B:416:LYS:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:ILE:HD13	1:D:501:HIS:HB3	1.86	0.55
1:B:371:THR:HG21	3:B:2082:HOH:O	2.06	0.55
1:D:547:HIS:O	1:D:548:ARG:HB2	2.08	0.54
1:B:348:ASN:ND2	1:B:352:ARG:HE	2.06	0.54
1:D:362:LYS:HE2	1:D:368:VAL:HG12	1.90	0.54
1:A:403:LEU:HD12	1:A:409:LEU:HD13	1.90	0.54
1:A:307:ALA:N	3:A:1082:HOH:O	2.41	0.54
1:C:369:ASP:HB2	1:C:474:HIS:CE1	2.39	0.54
1:A:515:ARG:NH1	3:A:1039:HOH:O	2.40	0.53
1:C:348:ASN:ND2	1:C:352:ARG:HE	2.05	0.53
1:D:358:ILE:HG23	1:D:544:LEU:HD13	1.91	0.53
1:A:362:LYS:HG3	1:A:547:HIS:CE1	2.44	0.53
1:D:380:GLU:OE2	1:D:537:TYR:CD2	2.63	0.52
1:A:311:THR:HG22	1:A:313:ASP:H	1.75	0.52
1:C:476:HIS:CD2	1:D:434:ARG:CZ	2.94	0.51
1:D:380:GLU:OE2	1:D:537:TYR:CE2	2.64	0.51
1:C:487:ILE:CD1	1:D:501:HIS:HB3	2.41	0.50
1:A:501:HIS:HD2	1:B:501:HIS:CD2	2.29	0.50
1:A:412:ARG:HG3	1:A:412:ARG:NH1	2.24	0.50
1:C:514:ILE:HA	1:C:517:MET:HE3	1.93	0.50
1:B:396:MET:O	1:B:436:ARG:HD3	2.12	0.50
1:A:412:ARG:HD2	1:A:425:PHE:CE1	2.48	0.49
1:B:497:LEU:O	1:B:501:HIS:ND1	2.45	0.49
1:C:329:SER:OG	1:C:345:LEU:HD13	2.13	0.49
1:D:369:ASP:HB2	1:D:474:HIS:HE1	1.78	0.49
1:D:362:LYS:HE3	1:D:368:VAL:HG12	1.94	0.48
1:C:348:ASN:ND2	1:C:352:ARG:HH21	2.10	0.48
1:D:358:ILE:HG21	1:D:543:MET:HB3	1.95	0.48
1:C:476:HIS:HD2	1:D:434:ARG:CZ	2.27	0.48
1:D:481:LYS:NZ	3:D:4088:HOH:O	2.47	0.48
1:A:456:SER:HA	1:A:515:ARG:NH2	2.27	0.47
1:D:403:LEU:HD23	1:D:409:LEU:HD13	1.96	0.47
1:A:434:ARG:HA	1:A:437:MET:CG	2.44	0.47
1:B:467:LYS:O	1:B:467:LYS:HG2	2.14	0.47
1:B:393:TRP:CE3	1:B:396:MET:HE3	2.50	0.47
1:D:504:LEU:O	1:D:508:LEU:HG	2.14	0.47
1:C:434:ARG:HG2	1:C:510:ILE:HD11	1.97	0.46
1:A:411:ASP:H	1:A:414:GLN:HE21	1.63	0.46
1:B:393:TRP:CE3	1:B:396:MET:CE	2.99	0.46
1:A:501:HIS:CD2	1:B:501:HIS:CD2	3.04	0.45
1:A:501:HIS:CD2	1:B:501:HIS:NE2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ASP:CB	1:A:474:HIS:HE1	2.30	0.45
1:A:502:GLN:O	3:A:1013:HOH:O	2.21	0.45
1:D:308:LEU:HD12	1:D:308:LEU:N	2.32	0.45
1:C:411:ASP:CG	1:C:414:GLN:HE21	2.21	0.45
1:B:524:HIS:O	1:B:524:HIS:ND1	2.51	0.44
1:B:519:ASN:ND2	3:B:2006:HOH:O	2.50	0.44
1:B:421:MET:HG3	1:B:421:MET:O	2.17	0.44
1:D:415:GLY:HA3	1:D:425:PHE:CD2	2.52	0.44
1:C:402:LEU:HD12	1:C:425:PHE:CZ	2.52	0.44
1:C:398:HIS:CE1	3:C:3034:HOH:O	2.70	0.44
1:D:472:LYS:NZ	1:D:472:LYS:HB2	2.33	0.44
1:B:379:LEU:HD12	1:B:544:LEU:HD11	1.99	0.44
1:D:371:THR:HG22	1:D:373:HIS:H	1.83	0.43
1:A:477:ARG:CZ	3:A:1091:HOH:O	2.67	0.43
1:A:412:ARG:HD2	1:A:425:PHE:CD1	2.53	0.43
1:A:433:SER:O	1:A:437:MET:HG2	2.19	0.43
1:A:487:ILE:HD11	1:A:504:LEU:HD22	2.01	0.43
1:A:461:PHE:O	3:A:1095:HOH:O	2.21	0.43
1:C:326:ILE:HD12	3:C:3043:HOH:O	2.18	0.42
1:A:518:SER:O	1:A:522:MET:HB2	2.19	0.42
1:B:398:HIS:N	1:B:399:PRO:HD3	2.34	0.42
1:D:392:VAL:HG13	1:D:432:SER:HA	2.02	0.42
1:A:403:LEU:HD13	1:A:409:LEU:HD13	2.01	0.42
1:D:372:LEU:O	1:D:376:VAL:HG23	2.20	0.42
1:A:360:TRP:CZ3	1:A:386:ILE:HD13	2.54	0.42
1:B:356:HIS:HE1	3:B:2015:HOH:O	2.03	0.41
3:A:1022:HOH:O	1:C:466:LEU:HG	2.20	0.41
1:C:398:HIS:N	1:C:398:HIS:ND1	2.69	0.41
1:B:356:HIS:HD2	3:B:2032:HOH:O	2.02	0.41
1:C:371:THR:CG2	3:C:3044:HOH:O	2.68	0.41
1:C:523:GLU:OE2	3:C:3049:HOH:O	2.22	0.41
1:D:546:ALA:O	1:D:548:ARG:N	2.53	0.41
1:D:385:GLU:OE2	1:D:456:SER:OG	2.25	0.41
1:B:311:THR:HG22	1:B:314:GLN:CD	2.41	0.41
1:C:501:HIS:CB	3:C:3042:HOH:O	2.66	0.41
1:A:369:ASP:HB2	1:A:474:HIS:HE1	1.86	0.41
1:A:477:ARG:HD2	3:A:1091:HOH:O	2.21	0.41
1:A:372:LEU:HD21	1:A:541:LEU:HD11	2.02	0.41
1:D:466:LEU:C	1:D:466:LEU:HD22	2.40	0.40
1:C:476:HIS:CD2	1:D:434:ARG:NH1	2.89	0.40
1:B:312:ALA:HB3	1:B:488:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LYS:NZ	1:B:375:GLN:HE22	2.19	0.40
1:D:354:LEU:HD21	2:D:4001:AEJ:H551	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:TYR:OH	1:B:359:ASN:ND2[1_556]	2.14	0.06

## 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	216/254 (85%)	212 (98%)	4 (2%)	0	100	100
1	B	213/254 (84%)	205 (96%)	7 (3%)	1 (0%)	34	22
1	C	216/254 (85%)	214 (99%)	2 (1%)	0	100	100
1	D	213/254 (84%)	207 (97%)	6 (3%)	0	100	100
All	All	858/1016 (84%)	838 (98%)	19 (2%)	1 (0%)	56	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	417	SER

### 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	201/229 (88%)	194 (96%)	7 (4%)	43	35
1	B	198/229 (86%)	182 (92%)	16 (8%)	15	7
1	C	201/229 (88%)	189 (94%)	12 (6%)	24	13
1	D	198/229 (86%)	184 (93%)	14 (7%)	18	10
All	All	798/916 (87%)	749 (94%)	49 (6%)	23	13

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

Mol	Chain	Res	Type
1	A	381	SER
1	A	410	LEU
1	A	412	ARG
1	A	436	ARG
1	A	477	ARG
1	A	492	LYS
1	A	512	SER
1	B	330	GLU
1	B	341	SER
1	B	368	VAL
1	B	371	THR
1	B	381	SER
1	B	397	GLU
1	B	416	LYS
1	B	417	SER
1	B	421	MET
1	B	464	SER
1	B	466	LEU
1	B	467	LYS
1	B	477	ARG
1	B	492	LYS
1	B	495	LEU
1	B	539	LEU
1	C	317	SER
1	C	358	ILE
1	C	370	LEU
1	C	398	HIS
1	C	412	ARG
1	C	417	SER
1	C	432	SER

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Mol	Chain	Res	Type
1	C	472	LYS
1	C	477	ARG
1	C	487	ILE
1	C	512	SER
1	C	536	LEU
1	D	308	LEU
1	D	320	LEU
1	D	341	SER
1	D	354	LEU
1	D	362	LYS
1	D	449	LYS
1	D	464	SER
1	D	466	LEU
1	D	468	SER
1	D	470	GLU
1	D	487	ILE
1	D	507	LEU
1	D	537	TYR
1	D	544	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	HIS
1	A	414	GLN
1	A	474	HIS
1	A	476	HIS
1	A	498	GLN
1	A	501	HIS
1	A	524	HIS
1	B	348	ASN
1	B	356	HIS
1	B	375	GLN
1	B	413	ASN
1	B	474	HIS
1	B	476	HIS
1	B	488	HIS
1	B	506	GLN
1	B	519	ASN
1	C	314	GLN
1	C	348	ASN
1	C	414	GLN

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Mol	Chain	Res	Type
1	C	455	ASN
1	C	474	HIS
1	C	476	HIS
1	D	474	HIS
1	D	519	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	AEJ	A	1001	-	38,38,38	1.23	3 (7%)	48,54,54	1.92	12 (25%)
2	AEJ	B	2001	-	38,38,38	1.27	4 (10%)	48,54,54	1.55	9 (18%)
2	AEJ	C	3001	-	38,38,38	1.43	7 (18%)	48,54,54	1.76	8 (16%)
2	AEJ	D	4001	-	38,38,38	0.94	2 (5%)	48,54,54	1.64	13 (27%)

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	AEJ	A	1001	-	-	0/12/45/45	0/6/6/6
2	AEJ	B	2001	-	-	0/12/45/45	0/6/6/6
2	AEJ	C	3001	-	-	0/12/45/45	0/6/6/6
2	AEJ	D	4001	-	-	0/12/45/45	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3001	AEJ	C34-C24	-3.38	1.48	1.51
2	B	2001	AEJ	C27-N26	-3.37	1.42	1.46
2	A	1001	AEJ	C27-N26	-3.27	1.43	1.46
2	A	1001	AEJ	C34-C24	-2.99	1.48	1.51
2	C	3001	AEJ	C27-N26	-2.77	1.43	1.46
2	C	3001	AEJ	C30-C33	-2.09	1.47	1.51
2	D	4001	AEJ	C17-C15	2.08	1.42	1.38
2	A	1001	AEJ	C47-C45	2.12	1.43	1.38
2	C	3001	AEJ	C47-C45	2.20	1.43	1.38
2	C	3001	AEJ	O42-C39	2.26	1.42	1.37
2	B	2001	AEJ	C19-C24	2.43	1.55	1.52
2	D	4001	AEJ	C19-C24	2.62	1.55	1.52
2	C	3001	AEJ	C35-C37	2.68	1.43	1.38
2	B	2001	AEJ	C8-N7	2.75	1.50	1.46
2	B	2001	AEJ	C17-C15	2.94	1.44	1.38
2	C	3001	AEJ	C22-C14	3.09	1.45	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	AEJ	C19-C24-C34	-7.25	100.04	112.62
2	C	3001	AEJ	C19-C24-C34	-6.93	100.60	112.62
2	B	2001	AEJ	C19-C24-C34	-4.62	104.61	112.62
2	A	1001	AEJ	C58-C61-C64	-4.36	102.64	111.26
2	D	4001	AEJ	C19-C24-C34	-3.33	106.85	112.62
2	B	2001	AEJ	C15-C14-C22	-2.87	113.16	119.13
2	D	4001	AEJ	C15-C14-C22	-2.71	113.50	119.13
2	D	4001	AEJ	C8-N7-C4	-2.70	107.62	113.30
2	D	4001	AEJ	C64-N1-C11	-2.69	105.23	110.37
2	B	2001	AEJ	C58-C61-C64	-2.66	106.00	111.26
2	D	4001	AEJ	C27-N26-C44	-2.52	110.21	117.37
2	B	2001	AEJ	C61-C64-N1	-2.48	106.89	111.15
2	A	1001	AEJ	C15-C14-C22	-2.40	114.14	119.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4001	AEJ	C30-C33-C40	-2.40	115.09	119.84
2	D	4001	AEJ	C17-C19-C20	-2.39	115.25	118.31
2	A	1001	AEJ	C64-N1-C11	-2.38	105.82	110.37
2	C	3001	AEJ	C15-C14-C22	-2.07	114.83	119.13
2	C	3001	AEJ	C8-N7-C4	-2.07	108.96	113.30
2	C	3001	AEJ	C61-C64-N1	-2.05	107.64	111.15
2	A	1001	AEJ	C61-C64-N1	-2.01	107.69	111.15
2	A	1001	AEJ	C22-C14-N7	2.04	124.12	121.38
2	A	1001	AEJ	C20-C19-C24	2.05	124.56	120.77
2	A	1001	AEJ	C4-C2-N1	2.07	110.71	108.50
2	A	1001	AEJ	C51-C53-C44	2.09	122.53	119.69
2	D	4001	AEJ	C22-C20-C19	2.19	123.46	121.20
2	D	4001	AEJ	C20-C22-C14	2.25	123.27	120.36
2	A	1001	AEJ	C11-C8-N7	2.35	115.28	110.63
2	D	4001	AEJ	C4-C2-N1	2.41	111.07	108.50
2	C	3001	AEJ	C27-C30-C33	2.51	114.98	111.20
2	D	4001	AEJ	C27-C30-C33	2.59	115.10	111.20
2	B	2001	AEJ	C27-C30-C33	2.62	115.15	111.20
2	A	1001	AEJ	C17-C15-C14	2.64	123.78	120.36
2	B	2001	AEJ	C17-C15-C14	2.75	123.92	120.36
2	B	2001	AEJ	C15-C14-N7	2.78	125.12	121.38
2	C	3001	AEJ	C4-C2-N1	2.80	111.48	108.50
2	B	2001	AEJ	C11-C8-N7	2.90	116.37	110.63
2	D	4001	AEJ	C30-C27-N26	2.90	118.22	111.53
2	B	2001	AEJ	C22-C20-C19	2.92	124.21	121.20
2	C	3001	AEJ	C2-C4-N7	3.11	114.28	110.62
2	D	4001	AEJ	C15-C14-N7	3.49	126.08	121.38
2	C	3001	AEJ	C11-C8-N7	3.79	118.14	110.63
2	A	1001	AEJ	C27-C30-C33	5.67	119.74	111.20

There are no chirality outliers.

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
2	A	1001	AEJ	1	0
2	D	4001	AEJ	1	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	224/254 (88%)	-0.12	3 (1%) 79 83	24, 43, 58, 73	1 (0%)
1	B	221/254 (87%)	0.18	14 (6%) 23 26	27, 44, 73, 92	0
1	C	224/254 (88%)	0.01	9 (4%) 42 48	25, 45, 65, 81	1 (0%)
1	D	221/254 (87%)	0.09	13 (5%) 26 29	23, 42, 64, 80	0
All	All	890/1016 (87%)	0.04	39 (4%) 38 43	23, 43, 67, 92	2 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	464	SER	8.5
1	B	418	VAL	5.9
1	B	417	SER	5.7
1	D	547	HIS	5.5
1	B	547	HIS	4.7
1	B	420	GLY	4.3
1	D	418	VAL	4.1
1	B	546	ALA	3.9
1	B	548	ARG	3.7
1	B	535	PRO	3.7
1	C	419	GLU	3.4
1	C	307	ALA	3.4
1	A	412	ARG	3.2
1	B	419	GLU	3.1
1	D	330	GLU	3.1
1	D	341	SER	3.0
1	C	464	SER	3.0
1	C	417	SER	3.0
1	D	416	LYS	3.0
1	D	417	SER	2.8
1	C	420	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	537	TYR	2.7
1	A	548	ARG	2.7
1	B	539	LEU	2.7
1	D	437	MET	2.7
1	D	419	GLU	2.7
1	B	437	MET	2.6
1	B	497	LEU	2.6
1	C	548	ARG	2.5
1	A	464	SER	2.4
1	C	330	GLU	2.3
1	D	535	PRO	2.3
1	D	548	ARG	2.2
1	C	373	HIS	2.1
1	D	542	GLU	2.1
1	C	341	SER	2.1
1	D	309	SER	2.1
1	B	537	TYR	2.1
1	B	524	HIS	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(Å <sup>2</sup> )	Q<0.9
2	AEJ	A	1001	33/33	0.95	0.11	-0.20	28,33,36,36	0
2	AEJ	D	4001	33/33	0.95	0.11	-0.47	30,34,43,43	0
2	AEJ	B	2001	33/33	0.95	0.10	-0.57	25,34,43,46	0
2	AEJ	C	3001	33/33	0.95	0.09	-0.60	26,31,37,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.