



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:32 pm GMT

PDB ID : 1A52  
Title : ESTROGEN RECEPTOR ALPHA LIGAND-BINDING DOMAIN COM-  
PLEXED TO ESTRADIOL  
Authors : Tanenbaum, D.M.; Wang, Y.; Sigler, P.B.  
Deposited on : 1998-02-19  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

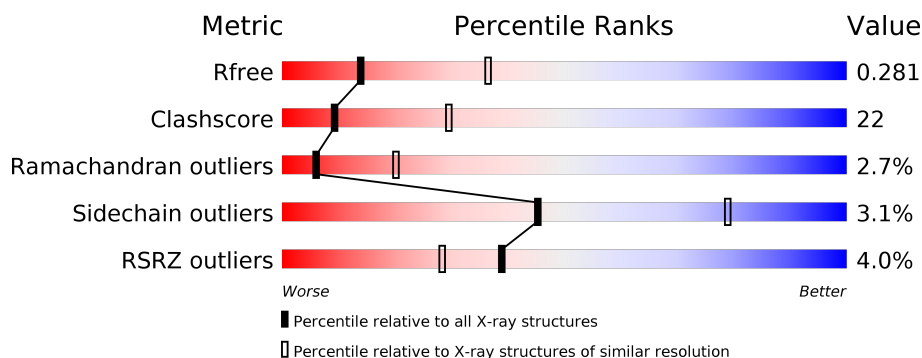
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	258	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>37%</div> <div>• 7%</div> </div> </div>
1	B	258	<div> <div>5%</div> <div> <div></div> <div>55%</div> <div>34%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3901 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.

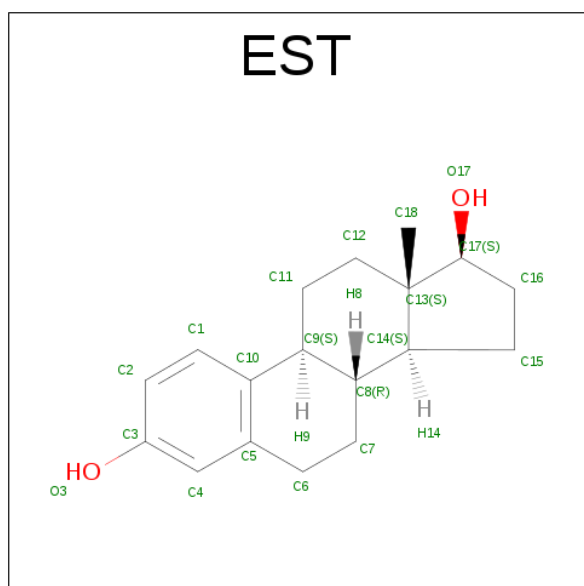
- Molecule 1 is a protein called ESTROGEN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	2	0
			1921	1231	325	346	19			
1	B	240	Total	C	N	O	S	0	1	0
			1904	1220	325	340	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	GLU	GLN	CONFLICT	UNP P03372
B	502	GLU	GLN	CONFLICT	UNP P03372

- Molecule 2 is ESTRADIOL (three-letter code: EST) (formula: C<sub>18</sub>H<sub>24</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	18	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			20	18	2		

- Molecule 3 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Au	0	0
			3	3		
3	A	3	Total	Au	0	0
			3	3		

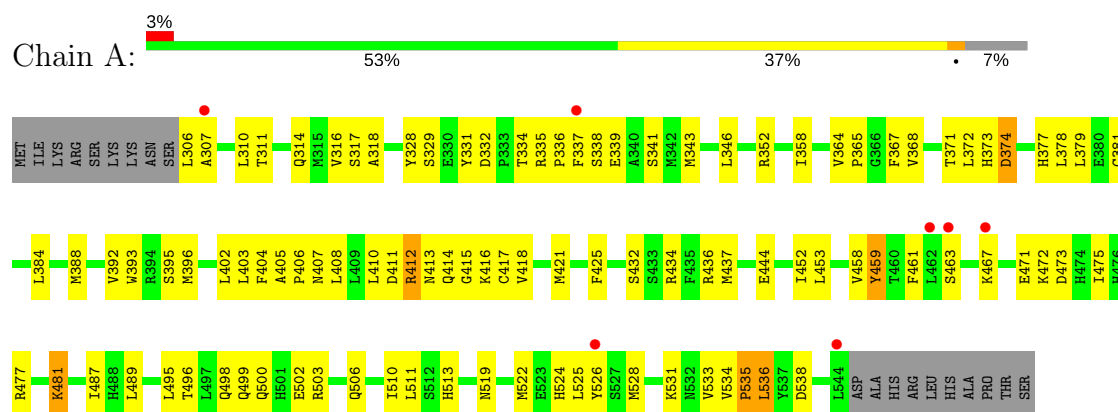
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	20	Total	O	0	0
			20	20		

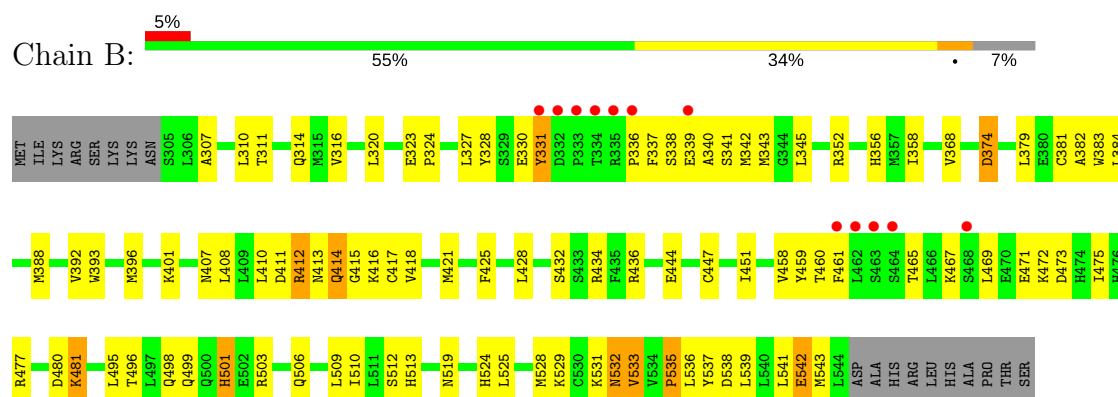
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: ESTROGEN RECEPTOR



#### • Molecule 1: ESTROGEN RECEPTOR



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.00Å 147.00Å 168.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 46.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.7 (50.00-2.80) 93.6 (46.28-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.08 (at 2.81Å)	Xtriage
Refinement program	CNS 0.3A	Depositor
R, $R_{free}$	0.223 , 0.274 0.235 , 0.281	Depositor DCC
$R_{free}$ test set	1639 reflections (10.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.5	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3901	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

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	0.60	0/1958	0.78	0/2647
1	B	0.63	0/1940	0.81	0/2623
All	All	0.61	0/3898	0.80	0/5270

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	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	459	TYR	Sidechain

### 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	1921	0	1957	89	0
1	B	1904	0	1944	91	0
2	A	20	0	24	1	0
2	B	20	0	24	1	0
3	A	3	0	0	1	0
3	B	3	0	0	1	0
4	A	10	0	0	2	0
4	B	20	0	0	2	0
All	All	3901	0	3949	172	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 22.

All (172) 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:519:ASN:HD22	1:B:519:ASN:ND2	1.62	0.96
1:A:519:ASN:ND2	1:B:519:ASN:HD22	1.65	0.93
1:A:374:ASP:OD2	1:A:471:GLU:HG2	1.71	0.88
1:B:535:PRO:HB2	1:B:539:LEU:HG	1.58	0.84
1:A:338:SER:H	1:A:341:SER:HB3	1.40	0.84
1:B:481:LYS:HE3	1:B:481:LYS:HA	1.61	0.82
1:A:381:CYS:HB2	4:A:559:HOH:O	1.80	0.81
1:A:519:ASN:HD22	1:B:519:ASN:HD22	0.84	0.81
1:B:337:PHE:HB3	1:B:417:CYS:SG	2.22	0.79
1:B:381:CYS:SG	3:B:13:AU:AU	2.10	0.78
1:B:338:SER:H	1:B:341:SER:HB3	1.49	0.76
1:A:481:LYS:HE3	1:A:481:LYS:HA	1.69	0.75
1:A:328:TYR:HB3	1:A:407:ASN:HD21	1.52	0.74
1:A:381:CYS:SG	3:A:3:AU:AU	2.15	0.74
1:A:332:ASP:OD2	1:A:334:THR:HB	1.87	0.73
1:B:328:TYR:HB3	1:B:407:ASN:HD21	1.52	0.72
1:A:335:ARG:HG3	1:A:336:PRO:HD2	1.73	0.71
1:B:528:MET:HB3	4:B:46:HOH:O	1.90	0.70
1:B:374:ASP:OD2	1:B:471:GLU:HG2	1.92	0.70
1:B:418:VAL:HG21	1:B:421:MET:HE3	1.73	0.69
1:A:535:PRO:O	1:A:536:LEU:HB2	1.93	0.69
1:A:410:LEU:N	1:A:410:LEU:HD12	2.07	0.68
1:A:306:LEU:N	1:A:306:LEU:HD12	2.08	0.68
1:B:330:GLU:HG2	1:B:352:ARG:NH2	2.10	0.66
1:B:535:PRO:HB3	1:B:538:ASP:CB	2.26	0.66
1:B:458:VAL:HG11	1:B:475:ILE:HG21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:MET:HG2	1:A:421:MET:O	1.99	0.62
1:B:396:MET:CE	1:B:436:ARG:HA	2.30	0.62
1:A:393:TRP:O	1:A:396:MET:HG3	1.99	0.62
1:A:358:ILE:HD13	1:A:379:LEU:HD13	1.80	0.61
1:A:513:HIS:CE1	1:B:459:TYR:HB2	2.35	0.61
1:A:307:ALA:HA	1:A:310:LEU:HD13	1.81	0.61
1:A:533:VAL:HG13	1:A:534:VAL:N	2.16	0.60
1:B:392:VAL:HG13	1:B:432:SER:HA	1.82	0.60
1:A:377:HIS:HD2	1:A:461:PHE:CE1	2.18	0.60
1:B:408:LEU:HD11	1:B:410:LEU:HD11	1.83	0.59
1:A:459:TYR:HB2	1:B:513:HIS:CE1	2.37	0.59
1:B:396:MET:HE3	1:B:436:ARG:HA	1.83	0.59
1:B:529:LYS:O	1:B:533:VAL:HG21	2.02	0.59
1:A:328:TYR:HB3	1:A:407:ASN:ND2	2.16	0.59
1:B:465:THR:O	1:B:469:LEU:HD13	2.03	0.58
1:A:528:MET:O	1:A:531:LYS:O	2.22	0.58
1:B:416:LYS:C	1:B:418:VAL:H	2.06	0.58
1:B:340:ALA:HB2	1:B:532:ASN:HD21	1.69	0.58
1:A:396:MET:CE	1:A:436:ARG:HA	2.34	0.57
1:A:413:ASN:O	1:A:415:GLY:N	2.37	0.57
1:A:395:SER:OG	1:A:402:LEU:HA	2.04	0.57
1:A:525:LEU:HD13	2:A:1:EST:H183	1.86	0.57
1:B:415:GLY:C	1:B:417:CYS:H	2.08	0.57
1:A:329:SER:HB3	1:A:407:ASN:OD1	2.05	0.56
1:B:408:LEU:CD1	1:B:410:LEU:HD11	2.35	0.56
1:B:410:LEU:N	1:B:410:LEU:HD12	2.20	0.56
1:B:339:GLU:HG2	1:B:418:VAL:HA	1.86	0.56
1:A:408:LEU:CD1	1:A:410:LEU:HD11	2.36	0.56
1:B:328:TYR:HB3	1:B:407:ASN:ND2	2.19	0.56
1:B:413:ASN:C	1:B:415:GLY:H	2.09	0.55
1:B:461:PHE:HB2	1:B:472:LYS:HE2	1.88	0.55
1:B:368:VAL:O	1:B:368:VAL:HG12	2.06	0.55
1:A:413:ASN:C	1:A:415:GLY:H	2.09	0.55
1:A:310:LEU:HA	1:A:314:GLN:OE1	2.07	0.54
1:B:328:TYR:HD2	1:B:407:ASN:HD22	1.54	0.54
1:A:410:LEU:CD1	1:A:410:LEU:N	2.70	0.54
1:A:332:ASP:CG	1:A:334:THR:HB	2.28	0.54
1:B:338:SER:O	1:B:341:SER:N	2.41	0.54
1:A:339:GLU:HA	1:A:417:CYS:O	2.08	0.54
1:A:335:ARG:CG	1:A:336:PRO:HD2	2.37	0.54
1:A:338:SER:N	1:A:341:SER:HB3	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLY:C	1:B:417:CYS:N	2.60	0.53
1:A:416:LYS:C	1:A:418:VAL:H	2.12	0.53
1:A:495:LEU:HB3	1:A:499:GLN:HB2	1.90	0.53
1:B:331:TYR:HB3	1:B:345:LEU:HD11	1.90	0.53
1:A:377:HIS:HD2	1:A:461:PHE:CD1	2.25	0.53
1:B:495:LEU:HB3	1:B:499:GLN:HB2	1.90	0.53
1:A:368:VAL:HG12	1:A:368:VAL:O	2.07	0.53
1:A:463:SER:HB3	1:A:472:LYS:HE3	1.90	0.53
1:A:467:LYS:O	1:A:471:GLU:HB2	2.09	0.52
1:A:473:ASP:O	1:A:477:ARG:HG3	2.09	0.52
1:B:340:ALA:CB	1:B:532:ASN:HD21	2.22	0.52
1:A:408:LEU:HD11	1:A:410:LEU:HD11	1.90	0.52
1:A:413:ASN:C	1:A:415:GLY:N	2.63	0.51
1:B:413:ASN:O	1:B:415:GLY:N	2.43	0.51
1:B:311:THR:OG1	1:B:314:GLN:HG3	2.11	0.51
1:A:338:SER:O	1:A:341:SER:N	2.44	0.50
1:B:413:ASN:C	1:B:415:GLY:N	2.64	0.50
1:B:496:THR:OG1	1:B:499:GLN:HG3	2.12	0.50
1:A:458:VAL:HG11	1:A:475:ILE:HG21	1.93	0.50
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.93	0.50
1:A:452:ILE:HD11	1:A:511:LEU:HD22	1.94	0.50
1:B:447:CYS:O	1:B:451:ILE:HG13	2.12	0.50
1:A:498:GLN:O	1:A:502:GLU:HG3	2.12	0.49
1:B:467:LYS:O	1:B:471:GLU:HB2	2.12	0.49
1:B:528:MET:HE2	4:B:46:HOH:O	2.10	0.49
1:B:471:GLU:HA	1:B:471:GLU:OE1	2.12	0.49
1:A:338:SER:O	1:A:339:GLU:C	2.49	0.49
1:B:310:LEU:CD1	1:B:310:LEU:H	2.24	0.49
1:B:328:TYR:HD2	1:B:407:ASN:ND2	2.11	0.49
1:B:535:PRO:O	1:B:537:TYR:N	2.46	0.48
1:B:458:VAL:CG1	1:B:475:ILE:HG21	2.41	0.48
1:B:418:VAL:HG11	1:B:421:MET:HE2	1.95	0.47
1:B:498:GLN:O	1:B:501[A]:HIS:CD2	2.68	0.47
1:A:384:LEU:O	1:A:388:MET:HG3	2.14	0.47
1:B:421:MET:HG2	1:B:421:MET:O	2.13	0.47
1:A:418:VAL:HG11	1:A:421:MET:CE	2.45	0.46
1:A:328:TYR:HD2	1:A:407:ASN:ND2	2.13	0.46
1:B:506:GLN:O	1:B:510:ILE:HG13	2.15	0.46
1:B:327:LEU:HD11	1:B:356:HIS:HD2	1.81	0.46
1:A:533:VAL:HG13	1:A:534:VAL:H	1.78	0.46
1:B:410:LEU:N	1:B:410:LEU:CD1	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ILE:HG13	1:B:501[A]:HIS:ND1	2.30	0.46
1:B:418:VAL:HG11	1:B:421:MET:CE	2.46	0.46
1:B:343:MET:HG3	1:B:528:MET:HE1	1.98	0.46
1:B:310:LEU:HA	1:B:314:GLN:OE1	2.16	0.45
1:B:414:GLN:O	1:B:417:CYS:HB3	2.15	0.45
1:A:352:ARG:NH1	4:A:564:HOH:O	2.49	0.45
1:B:495:LEU:N	1:B:495:LEU:HD12	2.32	0.45
1:A:418:VAL:HG11	1:A:421:MET:HE2	1.99	0.44
1:A:418:VAL:HG21	1:A:421:MET:HE3	1.98	0.44
1:A:506:GLN:O	1:A:510:ILE:HG13	2.18	0.44
1:B:509:LEU:O	1:B:512:SER:HB3	2.17	0.44
1:B:316:VAL:HG12	1:B:320:LEU:HD12	1.98	0.44
1:A:364:VAL:HA	1:A:365:PRO:HD3	1.81	0.44
1:A:522:MET:HE3	1:A:526:TYR:CE2	2.53	0.44
1:B:393:TRP:O	1:B:396:MET:HG3	2.18	0.44
1:B:382:ALA:O	1:B:383:TRP:C	2.54	0.44
1:B:401:LYS:HG2	1:B:411:ASP:HB3	2.00	0.44
1:A:329:SER:C	1:A:331:TYR:N	2.65	0.43
1:A:371:THR:O	1:A:372:LEU:C	2.55	0.43
1:A:392:VAL:HG13	1:A:432:SER:HA	2.00	0.43
1:A:317:SER:O	1:A:318:ALA:C	2.55	0.43
1:A:329:SER:O	1:A:331:TYR:N	2.48	0.43
1:A:536:LEU:C	1:A:538:ASP:N	2.70	0.43
1:B:358:ILE:HD13	1:B:379:LEU:HD13	2.00	0.43
1:B:444:GLU:CD	1:B:503:ARG:HH21	2.22	0.43
1:A:502:GLU:OE2	1:B:480:ASP:HB3	2.19	0.42
1:B:524:HIS:O	1:B:528:MET:HG2	2.19	0.42
1:A:377:HIS:CD2	1:A:461:PHE:CD1	3.05	0.42
1:B:411:ASP:O	1:B:412:ARG:C	2.57	0.42
1:B:428:LEU:HD23	1:B:428:LEU:HA	1.92	0.42
1:B:473:ASP:O	1:B:477:ARG:HG3	2.19	0.42
1:A:371:THR:HG22	1:A:373:HIS:N	2.35	0.42
1:A:524:HIS:O	1:A:528:MET:HG2	2.20	0.42
1:B:342:MET:O	1:B:345:LEU:N	2.53	0.42
1:B:396:MET:HE3	1:B:436:ARG:CA	2.49	0.42
1:B:541:LEU:O	1:B:542:GLU:O	2.38	0.42
1:A:496:THR:O	1:A:500:GLN:HG3	2.20	0.42
1:A:343:MET:HG3	1:A:528:MET:CE	2.50	0.42
1:A:346:LEU:HD22	1:A:404:PHE:CD2	2.55	0.42
1:A:411:ASP:O	1:A:412:ARG:C	2.57	0.42
1:B:339:GLU:HA	1:B:417:CYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:H	1:B:310:LEU:HD12	1.85	0.41
1:A:513:HIS:HE1	1:B:460:THR:HG23	1.84	0.41
1:B:525:LEU:HD13	2:B:2:EST:H183	2.00	0.41
1:B:343:MET:HG3	1:B:528:MET:CE	2.49	0.41
1:A:328:TYR:CE2	1:A:406:PRO:HB2	2.55	0.41
1:B:307:ALA:HA	1:B:310:LEU:HD13	2.02	0.41
1:B:327:LEU:HD11	1:B:356:HIS:CD2	2.55	0.41
1:A:311:THR:OG1	1:A:314:GLN:HG3	2.20	0.41
1:A:403:LEU:HD12	1:A:405:ALA:O	2.20	0.41
1:B:384:LEU:O	1:B:388:MET:HG3	2.20	0.41
1:A:378:LEU:HA	1:A:378:LEU:HD23	1.67	0.41
1:B:401:LYS:HE2	1:B:411:ASP:HB3	2.03	0.41
1:A:444:GLU:CD	1:A:503:ARG:HH21	2.22	0.41
1:A:403:LEU:CD1	1:A:405:ALA:O	2.69	0.40
1:A:534:VAL:HA	1:A:535:PRO:HD3	1.84	0.40
1:B:323:GLU:HA	1:B:324:PRO:HD2	1.91	0.40
1:B:327:LEU:HD13	1:B:352:ARG:HG2	2.02	0.40
1:B:401:LYS:HG2	1:B:411:ASP:CB	2.51	0.40
1:A:367:PHE:CD1	1:A:453:LEU:HD21	2.57	0.40
1:B:469:LEU:HD12	1:B:469:LEU:N	2.36	0.40
1:A:306:LEU:N	1:A:306:LEU:CD1	2.81	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	239/258 (93%)	220 (92%)	15 (6%)	4 (2%)	11	34
1	B	239/258 (93%)	215 (90%)	15 (6%)	9 (4%)	4	12
All	All	478/516 (93%)	435 (91%)	30 (6%)	13 (3%)	6	20

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	535	PRO
1	A	536	LEU
1	B	533	VAL
1	B	542	GLU
1	A	412	ARG
1	A	414	GLN
1	B	531	LYS
1	B	336	PRO
1	B	412	ARG
1	B	414	GLN
1	B	532	ASN
1	B	536	LEU
1	B	543	MET

### 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	216/233 (93%)	210 (97%)	6 (3%)	49	82
1	B	213/233 (91%)	205 (96%)	8 (4%)	38	72
All	All	429/466 (92%)	415 (97%)	14 (3%)	45	77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	PHE
1	A	374	ASP
1	A	425	PHE
1	A	434	ARG
1	A	437	MET
1	A	481	LYS
1	B	331	TYR
1	B	374	ASP
1	B	425	PHE
1	B	434	ARG

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Mol	Chain	Res	Type
1	B	481	LYS
1	B	501[A]	HIS
1	B	501[B]	HIS
1	B	535	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	HIS
1	A	359	ASN
1	A	377	HIS
1	A	439	ASN
1	A	455	ASN
1	A	498	GLN
1	A	513	HIS
1	B	356	HIS
1	B	359	ASN
1	B	375	GLN
1	B	407	ASN
1	B	439	ASN
1	B	455	ASN
1	B	498	GLN
1	B	513	HIS
1	B	519	ASN
1	B	532	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	EST	A	1	-	23,23,23	1.64	6 (26%)	36,36,36	0.83	0
2	EST	B	2	-	23,23,23	1.65	6 (26%)	36,36,36	0.91	1 (2%)

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	EST	A	1	-	-	0/0/40/40	0/4/4/4
2	EST	B	2	-	-	0/0/40/40	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	EST	C1-C10	2.18	1.42	1.39
2	B	2	EST	C1-C10	2.28	1.42	1.39
2	A	1	EST	C9-C8	2.30	1.57	1.54
2	A	1	EST	C4-C5	2.57	1.44	1.39
2	B	2	EST	C4-C5	2.58	1.44	1.39
2	B	2	EST	C16-C17	2.67	1.58	1.53
2	B	2	EST	C9-C8	2.81	1.57	1.54
2	A	1	EST	C4-C3	2.93	1.43	1.39
2	B	2	EST	C4-C3	2.95	1.43	1.39
2	A	1	EST	C16-C17	2.98	1.59	1.53
2	A	1	EST	C5-C10	3.63	1.46	1.39
2	B	2	EST	C5-C10	3.83	1.46	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	2	EST	C16-C17-C13	2.23	106.32	104.53

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	1	EST	1	0
2	B	2	EST	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	239/258 (92%)	0.03	7 (2%) 52 41	34, 56, 83, 85	0
1	B	240/258 (93%)	0.23	12 (5%) 30 20	27, 49, 85, 85	0
All	All	479/516 (92%)	0.13	19 (3%) 39 28	27, 54, 85, 85	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	464	SER	5.9
1	B	333	PRO	5.3
1	B	468	SER	5.3
1	B	462	LEU	5.0
1	B	463	SER	4.7
1	B	331	TYR	4.0
1	A	463	SER	3.7
1	B	332	ASP	3.6
1	A	467	LYS	3.4
1	B	335	ARG	3.3
1	A	307	ALA	2.8
1	B	461	PHE	2.6
1	A	337	PHE	2.3
1	B	334	THR	2.2
1	A	544	LEU	2.2
1	B	336	PRO	2.2
1	B	339	GLU	2.1
1	A	526	TYR	2.1
1	A	462	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EST	B	2	20/20	0.96	0.24	1.77	39,40,42,44	0
2	EST	A	1	20/20	0.97	0.20	0.11	44,46,47,47	0
3	AU	A	2	1/1	0.97	0.16	-	80,80,80,80	1
3	AU	B	13	1/1	0.99	0.20	-	72,72,72,72	1
3	AU	A	3	1/1	0.99	0.18	-	79,79,79,79	1
3	AU	B	15	1/1	0.96	0.12	-	85,85,85,85	1
3	AU	B	12	1/1	0.98	0.13	-	74,74,74,74	1
3	AU	A	5	1/1	0.86	0.12	-	85,85,85,85	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.