Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:42 PM GMT

PDB ID	:	1GWR
Title	:	HUMAN OESTROGEN RECEPTOR ALPHA LIGAND-BINDING DOMAIN IN COMPLEX WITH 17BETA-OESTRADIOL AND TIF2 NRBOX3 PEPTIDE
Authors	:	Pike, A.C.W.; Brzozowski, A.M.
Deposited on	:	2002-03-22
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

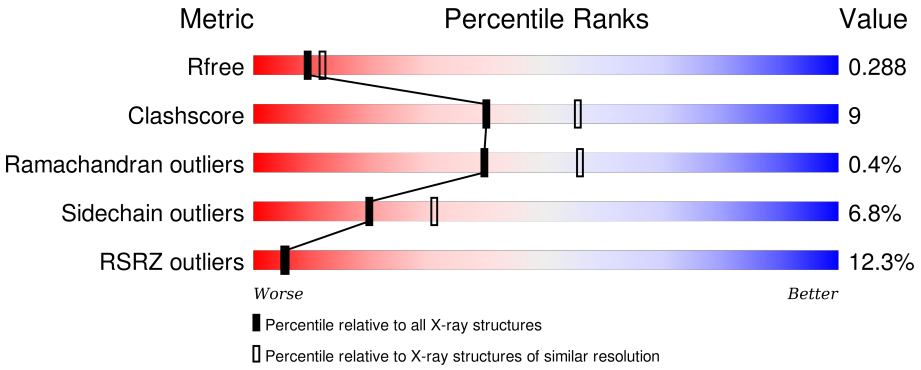
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 <=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	245	12% 67% 26%
1	B	245	12% 71% 22%
2	C	9	89% 11%
2	D	9	11% 67% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3987 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.

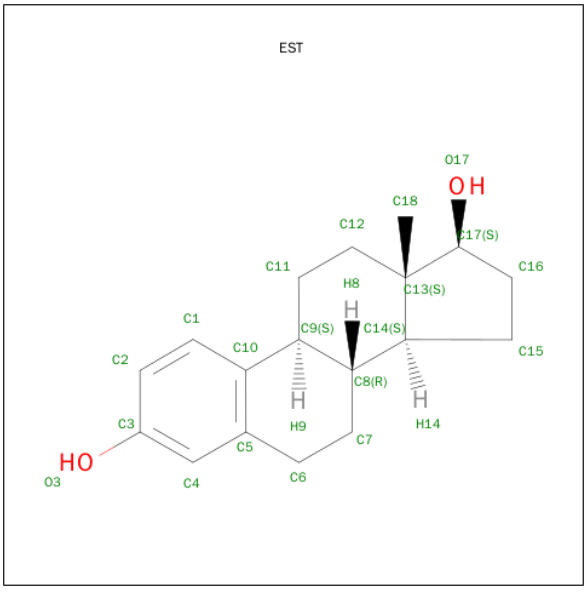
- Molecule 1 is a protein called OESTROGEN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	2	0
			1876	1201	322	334	19			
1	B	239	Total	C	N	O	S	0	2	0
			1880	1198	323	339	20			

- Molecule 2 is a protein called TRANSCRIPTION INTERMEDIARY FACTOR-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			70	47	10	13			
2	D	9	Total	C	N	O	0	0	0
			76	50	13	13			

- Molecule 3 is ESTRADIOL (three-letter code: EST) (formula: $C_{18}H_{24}O_2$).



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

- Molecule 4 is water.

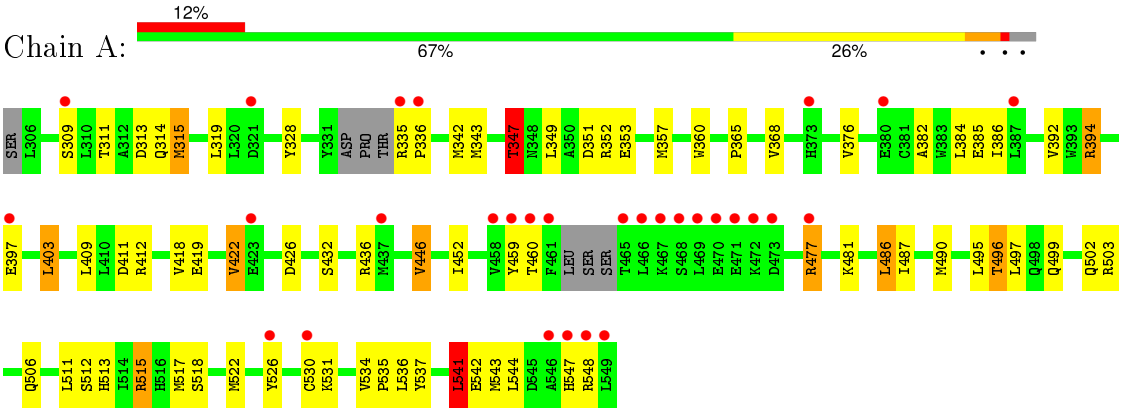
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	26	Total O 26 26	0	0
4	B	19	Total O 19 19	0	0

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.

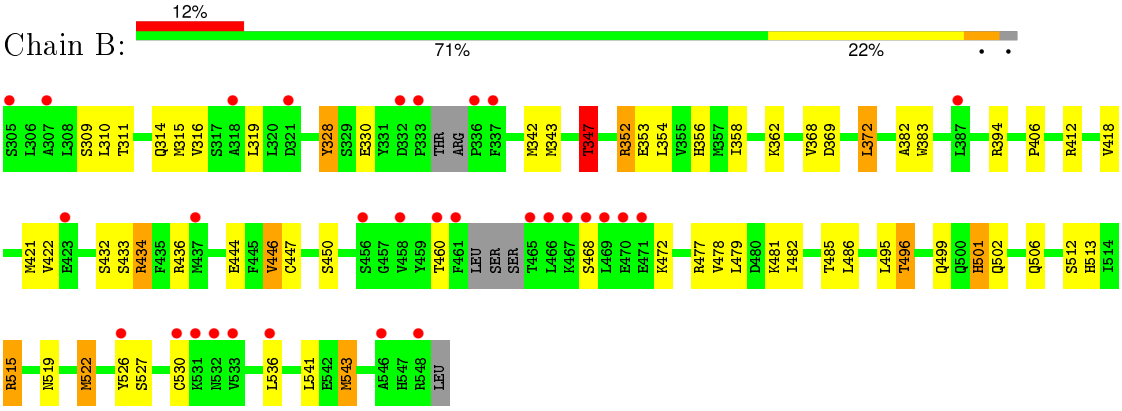
- Molecule 1: OESTROGEN RECEPTOR

Chain A:



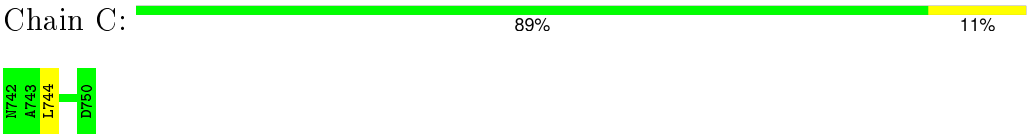
- Molecule 1: OESTROGEN RECEPTOR

Chain B:



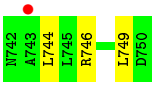
- Molecule 2: TRANSCRIPTION INTERMEDIARY FACTOR-2

Chain C:



- Molecule 2: TRANSCRIPTION INTERMEDIARY FACTOR-2

Chain D:


N742
A743
L744
L745
R746
L749
D750

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.31Å 90.54Å 59.23Å 90.00° 109.83° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 24.45 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.0 (25.00-2.40) 94.7 (24.45-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.225 , 0.288 0.224 , 0.288	Depositor DCC
R_{free} test set	1052 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 20664 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3987	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 12.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0/1920	1.58	25/2594 (1.0%)
1	B	0.60	0/1924	1.57	26/2600 (1.0%)
2	C	0.54	0/70	1.15	0/95
2	D	0.60	0/76	1.81	1/102 (1.0%)
All	All	0.61	0/3990	1.57	52/5391 (1.0%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	352	ARG	NE-CZ-NH1	-10.94	114.83	120.30
1	B	436	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	B	394	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	B	436	ARG	NE-CZ-NH1	10.24	125.42	120.30
2	D	746	ARG	NE-CZ-NH2	-10.03	115.29	120.30
1	A	352	ARG	CD-NE-CZ	9.86	137.41	123.60
1	A	394	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	B	436	ARG	CD-NE-CZ	9.17	136.44	123.60
1	A	313	ASP	CB-CG-OD2	9.03	126.42	118.30
1	A	503	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	394	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	515	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	347	THR	CA-CB-CG2	8.04	123.65	112.40
1	B	543	MET	CA-CB-CG	7.77	126.51	113.30
1	B	353	GLU	OE1-CD-OE2	-7.63	114.15	123.30
1	B	328	TYR	CB-CG-CD2	7.57	125.54	121.00
1	A	351	ASP	CB-CG-OD1	7.38	124.95	118.30
1	B	347	THR	N-CA-CB	-7.13	96.75	110.30
1	A	436	ARG	CD-NE-CZ	6.93	133.30	123.60
1	B	501	HIS	CB-CA-C	-6.59	97.21	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	347	THR	CA-CB-CG2	6.55	121.57	112.40
1	A	352	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	541	LEU	CA-CB-CG	6.52	130.30	115.30
1	B	352	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	B	512	SER	N-CA-CB	-6.27	101.10	110.50
1	A	328	TYR	CB-CG-CD1	6.14	124.69	121.00
1	A	436	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	422	VAL	CB-CA-C	-6.00	100.01	111.40
1	A	477	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	403	LEU	O-C-N	-5.70	113.58	122.70
1	B	446	VAL	CA-CB-CG1	5.70	119.45	110.90
1	A	446	VAL	CG1-CB-CG2	-5.59	101.95	110.90
1	B	382	ALA	CB-CA-C	-5.57	101.75	110.10
1	B	394	ARG	NH1-CZ-NH2	-5.55	113.29	119.40
1	B	412	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	B	356	HIS	CA-CB-CG	-5.48	104.28	113.60
1	B	412	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	A	347	THR	N-CA-CB	-5.47	99.91	110.30
1	A	486	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	B	515	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	526	TYR	CB-CG-CD1	5.35	124.21	121.00
1	A	503	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	486	LEU	CA-CB-CG	5.24	127.35	115.30
1	B	446	VAL	N-CA-CB	-5.18	100.11	111.50
1	B	460	THR	N-CA-CB	5.16	120.09	110.30
1	A	384	LEU	O-C-N	-5.13	114.49	122.70
1	B	519	ASN	N-CA-CB	5.13	119.83	110.60
1	B	434	ARG	CD-NE-CZ	5.05	130.68	123.60
1	B	369	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	352	ARG	NH1-CZ-NH2	-5.02	113.87	119.40
1	A	495	LEU	N-CA-CB	5.02	120.44	110.40
1	B	486	LEU	CB-CA-C	-5.02	100.67	110.20

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	1876	0	1888	42	0
1	B	1880	0	1884	33	0
2	C	70	0	69	3	0
2	D	76	0	80	3	0
3	A	20	0	24	0	0
3	B	20	0	24	0	0
4	A	26	0	0	0	0
4	B	19	0	0	0	0
All	All	3987	0	3969	70	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 9.

All (70) 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:496:THR:HG22	1:B:499:GLN:H	1.18	1.08
1:A:496:THR:HG22	1:A:499:GLN:H	1.41	0.83
1:B:319:LEU:HB3	1:B:446:VAL:CG1	2.13	0.78
1:A:335:ARG:N	1:A:336:PRO:HD2	1.99	0.78
1:A:319:LEU:HB3	1:A:446:VAL:CG1	2.15	0.77
1:B:343:MET:O	1:B:347:THR:HB	1.87	0.74
1:A:376:VAL:HG13	2:C:744:LEU:HD23	1.71	0.71
1:A:315:MET:HE3	1:A:365:PRO:HG2	1.73	0.70
1:B:496:THR:HB	1:B:499:GLN:OE1	1.91	0.69
1:A:543:MET:HE1	2:C:744:LEU:HD22	1.73	0.69
1:B:543:MET:HE3	2:D:744:LEU:HB2	1.76	0.68
1:A:357:MET:HE1	1:A:386:ILE:HB	1.75	0.67
1:A:502:GLN:O	1:A:506:GLN:HG3	1.94	0.67
1:A:319:LEU:HB3	1:A:446:VAL:HG12	1.76	0.67
1:A:543:MET:CE	2:C:744:LEU:HD22	2.27	0.64
1:A:522:MET:CE	1:A:544:LEU:HD12	2.29	0.63
1:A:335:ARG:N	1:A:336:PRO:CD	2.63	0.62
1:A:319:LEU:HB3	1:A:446:VAL:HG11	1.82	0.60
1:A:343:MET:O	1:A:347:THR:HB	2.02	0.60
1:B:496:THR:HG22	1:B:499:GLN:N	2.02	0.59
1:B:495:LEU:HB3	1:B:499:GLN:HB3	1.85	0.58
1:B:502:GLN:O	1:B:506:GLN:HG3	2.02	0.58
1:B:319:LEU:HB3	1:B:446:VAL:HG13	1.86	0.56
1:A:515:ARG:HH22	1:B:513[A]:HIS:CD2	2.24	0.55
1:A:349:LEU:O	1:A:353:GLU:HG3	2.09	0.53
1:A:392:VAL:HG13	1:A:432:SER:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:HIS:CE1	1:B:515:ARG:HH22	2.29	0.51
1:A:459:TYR:HE1	1:B:434:ARG:HD3	1.76	0.50
1:B:315:MET:HE2	1:B:482:ILE:HG12	1.93	0.50
1:B:383:TRP:HZ2	1:B:522:MET:HE1	1.77	0.49
1:B:543:MET:CE	2:D:744:LEU:HD22	2.42	0.49
1:A:342:MET:HE3	1:A:418:VAL:HG23	1.94	0.48
1:A:452:ILE:HD11	1:A:511:LEU:HD22	1.96	0.48
1:B:354:LEU:HD21	1:B:383:TRP:CE3	2.48	0.48
1:A:315:MET:CE	1:A:365:PRO:HG2	2.43	0.47
1:A:522:MET:HE1	1:A:544:LEU:HD12	1.94	0.47
1:A:496:THR:HB	1:A:499:GLN:OE1	2.14	0.47
1:A:347:THR:HG22	1:A:537:TYR:HE2	1.80	0.47
1:A:543:MET:HA	1:A:543:MET:HE2	1.97	0.47
1:A:419:GLU:OE1	1:A:531:LYS:NZ	2.48	0.47
1:B:311:THR:HG23	1:B:314:GLN:OE1	2.15	0.46
1:A:382:ALA:O	1:A:386:ILE:HG12	2.15	0.46
1:B:328:TYR:CZ	1:B:406:PRO:HG2	2.51	0.46
1:B:342:MET:HE2	1:B:418:VAL:HG23	1.97	0.46
1:A:486:LEU:O	1:A:490:MET:HG3	2.16	0.46
1:B:352:ARG:HD2	1:B:352:ARG:HH11	1.54	0.45
1:B:372:LEU:HD21	2:D:749:LEU:HD21	1.99	0.45
1:A:535:PRO:O	1:A:536:LEU:HD12	2.16	0.44
1:A:541:LEU:O	1:A:542:GLU:C	2.55	0.44
1:A:311:THR:HG23	1:A:314:GLN:OE1	2.16	0.44
1:B:310:LEU:O	1:B:481:LYS:HE3	2.18	0.44
1:B:444:GLU:O	1:B:447:CYS:HB2	2.18	0.44
1:B:526:TYR:CE1	1:B:530[A]:CYS:SG	3.11	0.44
1:A:412:ARG:NE	1:A:426:ASP:OD1	2.49	0.43
1:A:403:LEU:HD12	1:A:409:LEU:HD13	2.01	0.42
1:B:468:SER:O	1:B:472:LYS:HG3	2.19	0.42
1:A:342:MET:CE	1:A:418:VAL:HG23	2.50	0.42
1:A:403:LEU:CD1	1:A:409:LEU:HD13	2.50	0.41
1:A:487:ILE:HG13	1:B:501:HIS:ND1	2.36	0.41
1:A:513:HIS:O	1:A:517:MET:HG3	2.20	0.41
1:B:354:LEU:O	1:B:358:ILE:HG13	2.19	0.41
1:B:316:VAL:HG23	1:B:485:THR:CG2	2.51	0.41
1:B:421:MET:O	1:B:421:MET:HG3	2.20	0.41
1:A:515:ARG:NH2	1:B:513[A]:HIS:CD2	2.89	0.41
1:A:385:GLU:HG3	1:A:518:SER:HB2	2.04	0.40
1:B:479:LEU:HA	1:B:479:LEU:HD23	1.97	0.40
1:B:478:VAL:HG12	1:B:482:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ASP:O	1:A:412:ARG:C	2.60	0.40
1:A:547:HIS:O	1:A:548:ARG:C	2.60	0.40
1:B:536:LEU:HA	1:B:541:LEU:HD11	2.03	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	234/245 (96%)	226 (97%)	7 (3%)	1 (0%)	39	56
1	B	235/245 (96%)	228 (97%)	6 (3%)	1 (0%)	39	56
2	C	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
2	D	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	483/508 (95%)	465 (96%)	16 (3%)	2 (0%)	39	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	THR
1	B	330	GLU

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	206/221 (93%)	190 (92%)	16 (8%)	16 24
1	B	208/221 (94%)	195 (94%)	13 (6%)	22 35
2	C	7/8 (88%)	7 (100%)	0	100 100
2	D	8/8 (100%)	8 (100%)	0	100 100
All	All	429/458 (94%)	400 (93%)	29 (7%)	20 31

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	SER
1	A	315	MET
1	A	347	THR
1	A	360	TRP
1	A	368	VAL
1	A	394	ARG
1	A	397	GLU
1	A	422	VAL
1	A	477	ARG
1	A	481	LYS
1	A	496	THR
1	A	497	LEU
1	A	512	SER
1	A	530	CYS
1	A	534	VAL
1	A	541	LEU
1	B	309	SER
1	B	347	THR
1	B	362	LYS
1	B	368	VAL
1	B	372	LEU
1	B	422	VAL
1	B	432	SER
1	B	433	SER
1	B	450	SER
1	B	477	ARG
1	B	496	THR
1	B	522	MET
1	B	527	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	ASN
1	A	488	HIS
1	A	501	HIS

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

2 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	EST	A	600	-	23,23,23	1.16	1 (4%)	36,36,36	1.76	12 (33%)
3	EST	B	600	-	23,23,23	1.08	2 (8%)	36,36,36	1.96	11 (30%)

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	EST	A	600	-	-	0/0/40/40	0/4/4/4
3	EST	B	600	-	-	0/0/40/40	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	EST	C8-C14	-2.08	1.49	1.53
3	B	600	EST	C7-C8	2.11	1.57	1.53
3	A	600	EST	C1-C10	2.75	1.43	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	600	EST	C6-C7-C8	-5.04	103.27	110.67
3	A	600	EST	C7-C8-C14	-4.06	105.29	112.02
3	B	600	EST	C18-C13-C17	-3.80	103.26	109.49
3	A	600	EST	C12-C11-C9	-3.32	108.32	112.20
3	B	600	EST	C7-C6-C5	-3.09	107.05	112.86
3	B	600	EST	O17-C17-C13	-3.05	108.47	114.78
3	B	600	EST	C1-C2-C3	-2.90	116.51	119.87
3	A	600	EST	C3-C4-C5	-2.84	117.81	120.75
3	B	600	EST	C7-C8-C9	-2.75	106.58	109.26
3	A	600	EST	C15-C14-C13	-2.68	100.34	103.82
3	A	600	EST	C18-C13-C17	-2.63	105.19	109.49
3	A	600	EST	C6-C5-C4	-2.50	114.89	119.84
3	A	600	EST	C11-C12-C13	-2.29	108.75	112.84
3	B	600	EST	C11-C12-C13	-2.21	108.88	112.84
3	A	600	EST	C13-C14-C8	-2.14	111.02	114.37
3	A	600	EST	C16-C15-C14	-2.06	100.99	105.12
3	B	600	EST	C3-C4-C5	-2.02	118.66	120.75
3	B	600	EST	C2-C3-C4	2.20	122.71	120.19
3	A	600	EST	C11-C9-C10	2.25	116.41	113.72
3	A	600	EST	C18-C13-C12	2.34	114.53	110.54
3	A	600	EST	C4-C5-C10	2.49	122.89	119.52
3	B	600	EST	C12-C13-C14	2.78	111.83	107.31
3	B	600	EST	C11-C9-C10	2.79	117.05	113.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	238/245 (97%)	0.86	30 (12%) 5 5	17, 37, 85, 140	0
1	B	239/245 (97%)	0.88	30 (12%) 5 5	17, 35, 81, 140	0
2	C	9/9 (100%)	0.46	0 100 100	49, 52, 60, 66	0
2	D	9/9 (100%)	0.76	1 (11%) 7 7	36, 41, 50, 59	0
All	All	495/508 (97%)	0.86	61 (12%) 5 5	17, 36, 83, 140	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458	VAL	11.5
1	B	465	THR	9.2
1	A	468	SER	7.9
1	A	460	THR	7.9
1	B	468	SER	7.6
1	B	467	LYS	7.4
1	B	548	ARG	6.2
1	B	530[A]	CYS	6.0
1	A	335	ARG	5.4
1	B	307	ALA	5.0
1	A	465	THR	5.0
1	A	466	LEU	4.9
1	B	466	LEU	4.6
1	A	547	HIS	4.6
1	B	461	PHE	4.6
1	A	467	LYS	4.5
1	A	546	ALA	4.5
1	A	549	LEU	4.4
1	A	471	GLU	4.4
1	A	526	TYR	4.2
1	B	460	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	469	LEU	4.1
1	A	461	PHE	3.8
1	B	332	ASP	3.8
1	B	536	LEU	3.6
1	A	459	TYR	3.6
1	A	470	GLU	3.6
1	A	472	LYS	3.5
1	A	473	ASP	3.4
1	A	423	GLU	3.3
1	A	437	MET	3.1
1	A	477	ARG	3.0
1	B	321	ASP	3.0
1	B	532	ASN	3.0
1	B	333	PRO	2.9
1	A	387	LEU	2.9
1	B	470	GLU	2.8
1	B	471	GLU	2.8
1	A	321	ASP	2.8
1	B	336	PRO	2.8
2	D	743	ALA	2.7
1	B	437	MET	2.7
1	B	337	PHE	2.7
1	A	380	GLU	2.5
1	B	423	GLU	2.5
1	B	305	SER	2.4
1	A	530	CYS	2.4
1	A	336	PRO	2.4
1	A	548	ARG	2.4
1	B	533	VAL	2.4
1	B	318	ALA	2.4
1	A	309	SER	2.4
1	B	387	LEU	2.3
1	B	526	TYR	2.2
1	A	373[A]	HIS	2.2
1	B	469	LEU	2.2
1	B	458	VAL	2.1
1	B	531	LYS	2.1
1	B	456	SER	2.1
1	B	546	ALA	2.1
1	A	397	GLU	2.1

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^{th} 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	EST	A	600	20/20	0.86	0.28	1.80	19,24,25,26	0
3	EST	B	600	20/20	0.92	0.24	0.94	21,23,27,29	0

6.5 Other polymers (i)

There are no such residues in this entry.