



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:43 PM GMT

PDB ID : 2BJ4
Title : ESTROGEN RECEPTOR ALPHA LBD IN COMPLEX WITH A PHAGE-DISPLAY DERIVED PEPTIDE ANTAGONIST
Authors : Kong, E.; Heldring, N.; Gustafsson, J.A.; Treuter, E.; Hubbard, R.E.; Pike, A.C.W.
Deposited on : 2005-01-28
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

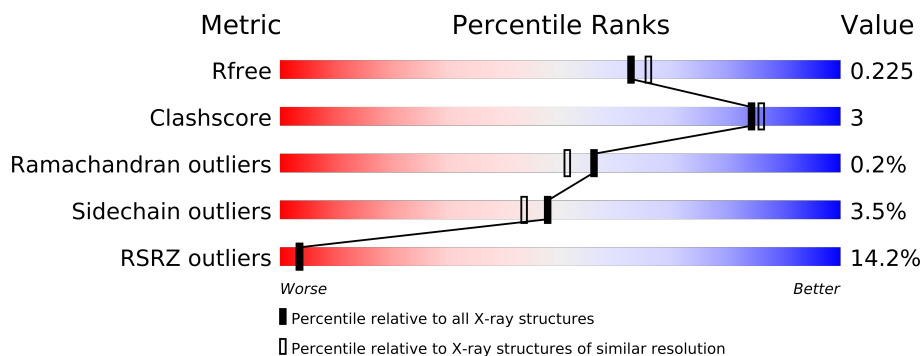
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	252	
2	B	252	
3	C	11	
3	D	11	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3922 atoms, of which 0 are hydrogen and 0 are deuterium.

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	218	Total	C	N	O	S	0	4	0
			1735	1110	297	311	17			

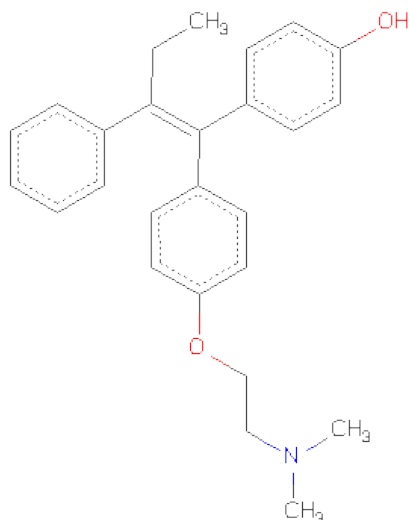
- Molecule 2 is a protein called ESTROGEN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	222	Total	C	N	O	S	0	4	0
			1764	1128	301	318	17			

- Molecule 3 is a protein called PEPTIDE ANTAGONIST.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			93	60	15	18			
3	D	11	Total	C	N	O	0	0	0
			93	60	15	18			

- Molecule 4 is 4-HYDROXYTAMOXIFEN (three-letter code: OHT) (formula: C₂₆H₂₉NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			29	26	1	2		
4	B	1	Total	C	N	O	0	0
			29	26	1	2		

- Molecule 5 is water.

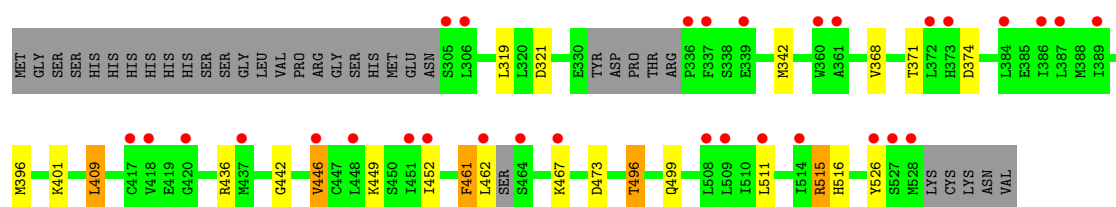
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total	O	0	0
			84	84		
5	B	90	Total	O	0	0
			90	90		
5	C	2	Total	O	0	0
			2	2		
5	D	3	Total	O	0	0
			3	3		

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 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.

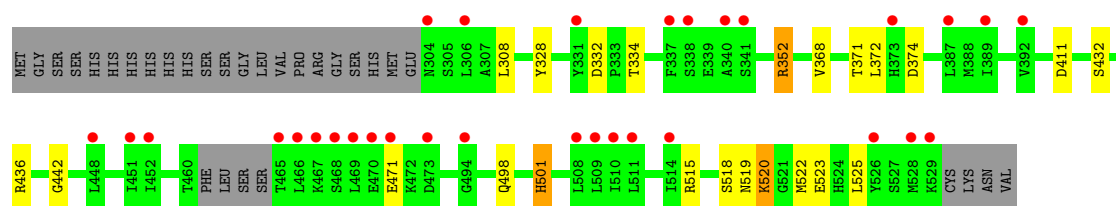
• Molecule 1: ESTROGEN RECEPTOR

Chain A: 



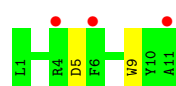
• Molecule 2: ESTROGEN RECEPTOR

Chain B: 



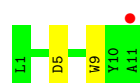
• Molecule 3: PEPTIDE ANTAGONIST

Chain C: 



• Molecule 3: PEPTIDE ANTAGONIST

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.76Å 98.76Å 105.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.99 – 2.00 28.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (28.99-2.00) 94.8 (28.93-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.187 , 0.219 0.195 , 0.225	Depositor DCC
R_{free} test set	1725 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34658 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3922	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.63	0/1782	0.81	5/2405 (0.2%)
2	B	0.62	1/1802 (0.1%)	0.78	8/2435 (0.3%)
3	C	0.57	0/96	0.77	1/128 (0.8%)
3	D	0.57	0/96	0.96	1/128 (0.8%)
All	All	0.62	1/3776 (0.0%)	0.80	15/5096 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	THR	CB-OG1	7.24	1.57	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ARG	NE-CZ-NH1	6.97	123.78	120.30
3	D	5	ASP	CB-CG-OD2	6.78	124.40	118.30
2	B	515	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	515	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	B	374	ASP	CB-CG-OD2	6.00	123.70	118.30
2	B	332	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	374	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	321	ASP	CB-CG-OD2	5.66	123.40	118.30
2	B	515	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	473	ASP	CB-CG-OD2	5.45	123.20	118.30
2	B	352	ARG	NE-CZ-NH1	5.11	122.85	120.30
3	C	5	ASP	CB-CG-OD2	5.08	122.87	118.30
2	B	352	ARG	NE-CZ-NH2	-5.03	117.79	120.30
2	B	411	ASP	CB-CG-OD2	5.00	122.80	118.30
2	B	436	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1735	0	1752	13	0
2	B	1764	0	1771	7	0
3	C	93	0	83	2	0
3	D	93	0	83	1	0
4	A	29	0	29	1	0
4	B	29	0	28	2	0
5	A	84	0	0	2	0
5	B	90	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	0	0
All	All	3922	0	3746	22	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (22) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:319:LEU:HB3	1:A:446:VAL:HG13	1.82	0.60
1:A:515:ARG:NH2	5:A:2081:HOH:O	2.33	0.60
4:A:1529:OHT:H91	4:A:1529:OHT:C6	2.36	0.55
1:A:516:HIS:HA	2:B:519:ASN:HD21	1.73	0.53
2:B:520:LYS:NZ	2:B:523:GLU:OE1	2.31	0.51
2:B:328:TYR:O	2:B:352:ARG:NH2	2.42	0.50
1:A:496:THR:HG23	5:A:2073:HOH:O	2.10	0.50
1:A:442:GLY:HA3	3:C:9:TRP:CD2	2.49	0.48
4:B:1530:OHT:H91	4:B:1530:OHT:C6	2.43	0.48
1:A:396:MET:O	1:A:436:ARG:HD3	2.15	0.47
1:A:496:THR:HG22	1:A:499:GLN:H	1.79	0.47
1:A:371:THR:HG21	1:A:467:LYS:HE2	1.98	0.46
1:A:442:GLY:HA3	3:C:9:TRP:CE3	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:442:GLY:HA3	3:D:9:TRP:CD2	2.53	0.43
4:B:1530:OHT:H231	4:B:1530:OHT:H253	1.68	0.42
1:A:461:PHE:O	1:A:462:LEU:CB	2.68	0.41
2:B:371:THR:HG23	2:B:471:GLU:OE2	2.19	0.41
2:B:498:GLN:HA	2:B:501[A]:HIS:CE1	2.55	0.41
1:A:401:LYS:HD2	1:A:409:LEU:HD22	2.01	0.41
1:A:371:THR:HG21	1:A:467:LYS:CE	2.51	0.41
1:A:452:ILE:HD11	1:A:511:LEU:HD22	2.03	0.41
2:B:518:SER:O	2:B:522:MET:HG2	2.21	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	216/252 (86%)	212 (98%)	3 (1%)	1 (0%)	38	29
2	B	221/252 (88%)	218 (99%)	3 (1%)	0	100	100
3	C	9/11 (82%)	9 (100%)	0	0	100	100
3	D	9/11 (82%)	9 (100%)	0	0	100	100
All	All	455/526 (86%)	448 (98%)	6 (1%)	1 (0%)	56	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	PHE

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	194/226 (86%)	187 (96%)	7 (4%)	47	42
2	B	194/225 (86%)	186 (96%)	8 (4%)	41	35
3	C	9/9 (100%)	9 (100%)	0	100	100
3	D	9/9 (100%)	9 (100%)	0	100	100
All	All	406/469 (87%)	391 (96%)	15 (4%)	48	40

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	MET
1	A	368	VAL
1	A	409	LEU
1	A	446	VAL
1	A	449	LYS
1	A	496	THR
1	A	526	TYR
2	B	308	LEU
2	B	368	VAL
2	B	372	LEU
2	B	432	SER
2	B	501[A]	HIS
2	B	501[B]	HIS
2	B	520	LYS
2	B	525	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	519	ASN
2	B	348	ASN
2	B	455	ASN
2	B	519	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CCS	B	417	2	9,9,10	7.30	3 (33%)	8,10,12	3.51	1 (12%)

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	CCS	B	417	2	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	417	CCS	O-C	18.72	1.24	1.11
2	B	417	CCS	CD-SG	-10.86	1.61	1.81
2	B	417	CCS	CA-C	3.03	1.54	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	417	CCS	CB-SG-CD	9.56	117.59	101.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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
4	OHT	A	1529	-	31,31,31	1.51	4 (12%)	41,41,41	1.30	5 (12%)
4	OHT	B	1530	-	31,31,31	1.48	4 (12%)	41,41,41	1.42	6 (14%)

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
4	OHT	A	1529	-	-	0/24/24/24	0/3/3/3
4	OHT	B	1530	-	-	0/24/24/24	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1529	OHT	C1-C7	-4.78	1.40	1.49
4	B	1530	OHT	C1-C7	-4.72	1.40	1.49
4	A	1529	OHT	C11-C8	-4.20	1.40	1.49
4	B	1530	OHT	C11-C8	-3.83	1.41	1.49
4	A	1529	OHT	C17-C7	-3.51	1.43	1.49
4	B	1530	OHT	C17-C7	-3.28	1.43	1.49
4	A	1529	OHT	C7-C8	2.12	1.40	1.34
4	B	1530	OHT	C7-C8	2.11	1.40	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1530	OHT	C12-C11-C8	3.83	126.52	121.00
4	B	1530	OHT	C16-C11-C8	-3.79	115.55	121.00
4	A	1529	OHT	C16-C11-C8	-3.39	116.13	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1530	OHT	C9-C8-C11	2.91	117.90	114.20
4	A	1529	OHT	C23-C24-N24	-2.65	107.57	114.72
4	B	1530	OHT	O20-C23-C24	-2.56	101.66	107.50
4	A	1529	OHT	C12-C11-C8	2.40	124.46	121.00
4	A	1529	OHT	C9-C8-C11	2.35	117.19	114.20
4	B	1530	OHT	C23-C24-N24	-2.27	108.59	114.72
4	A	1529	OHT	O20-C23-C24	-2.23	102.41	107.50
4	B	1530	OHT	C18-C19-C20	2.00	122.44	119.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/252 (86%)	0.83	31 (14%) 3 3	24, 30, 47, 56	0
2	B	222/252 (88%)	0.84	31 (13%) 3 3	23, 31, 46, 51	0
3	C	11/11 (100%)	1.48	3 (27%) 1 1	37, 39, 44, 46	0
3	D	11/11 (100%)	0.60	1 (9%) 9 9	30, 34, 38, 42	0
All	All	462/526 (87%)	0.84	66 (14%) 3 3	23, 31, 46, 56	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	468	SER	7.2
1	A	528	MET	6.1
2	B	340	ALA	5.9
2	B	304	ASN	5.7
1	A	526	TYR	5.0
1	A	417	CYS	4.5
2	B	465	THR	4.4
2	B	469	LEU	4.1
2	B	526	TYR	4.1
1	A	337	PHE	4.0
1	A	373	HIS	4.0
1	A	336	PRO	3.8
1	A	464	SER	3.8
2	B	511	LEU	3.7
3	C	11	ALA	3.6
1	A	527	SER	3.6
1	A	462	LEU	3.5
2	B	338	SER	3.4
2	B	452	ILE	3.4
2	B	467	LYS	3.4
2	B	466	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	508	LEU	3.2
2	B	471	GLU	3.2
1	A	511	LEU	3.1
2	B	451	ILE	3.1
2	B	331	TYR	3.0
2	B	306	LEU	2.9
2	B	448	LEU	2.9
2	B	470	GLU	2.9
1	A	451	ILE	2.9
1	A	420	GLY	2.8
2	B	373	HIS	2.8
2	B	508	LEU	2.7
1	A	448	LEU	2.7
1	A	389	ILE	2.7
3	C	6	PHE	2.7
1	A	305	SER	2.6
1	A	306	LEU	2.6
1	A	387	LEU	2.6
1	A	418	VAL	2.6
2	B	509	LEU	2.6
3	D	11	ALA	2.6
1	A	386	ILE	2.5
2	B	341	SER	2.5
2	B	337	PHE	2.5
1	A	452	ILE	2.5
1	A	339	GLU	2.5
2	B	529	LYS	2.4
2	B	392	VAL	2.4
1	A	514	ILE	2.4
2	B	389	ILE	2.4
2	B	473	ASP	2.4
2	B	514	ILE	2.4
1	A	372	LEU	2.4
1	A	384	LEU	2.4
1	A	437	MET	2.3
2	B	510	ILE	2.3
2	B	528	MET	2.3
1	A	446	VAL	2.2
1	A	360	TRP	2.2
2	B	387	LEU	2.2
2	B	494	GLY	2.2
3	C	4	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	467	LYS	2.1
1	A	509	LEU	2.0
1	A	361	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CCS	B	417	10/11	0.23	1.57	30,31,36,38	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	OHT	A	1529	29/29	0.15	-0.33	22,26,42,43	0
4	OHT	B	1530	29/29	0.12	-0.67	26,29,35,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.