



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:07 PM GMT

PDB ID : 2QXM  
Title : Crystal Structure of the Estrogen Receptor Alpha Ligand Binding Domain Complexed to Burned Meat Compound PhIP  
Authors : Nettles, K.W.; Bruning, J.B.; Gil, G.; Nowak, J.; Sharma, S.K.; Hahm, J.B.; Shi, Y.; Kulp, K.; Hochberg, R.B.; Zhou, H.; Katzenellenbogen, J.A.; Katzenellenbogen, B.S.; Kim, Y.; Joachmiak, A.; Greene, G.L.  
Deposited on : 2007-08-12  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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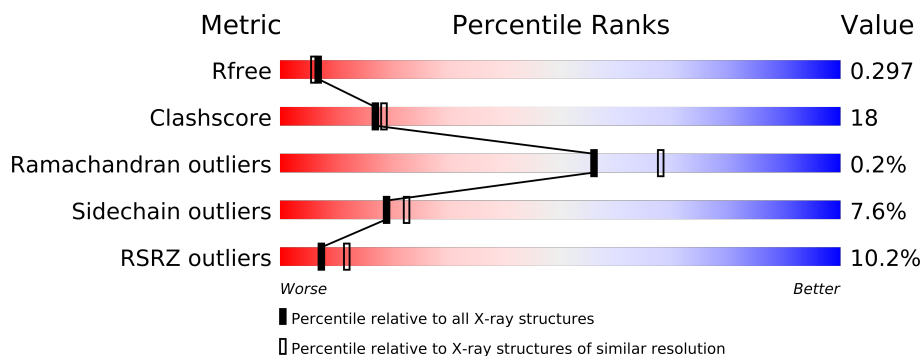
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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



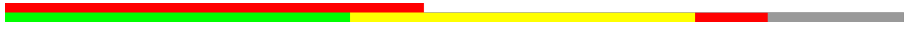
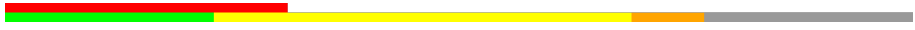
The reported resolution of this entry is 2.30 Å.

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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. 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	258	
1	B	258	
2	C	13	
2	D	13	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3997 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	233	Total	C	N	O	S	0	2	0
			1840	1184	309	328	19			
1	B	242	Total	C	N	O	S	0	6	0
			1941	1247	328	345	21			

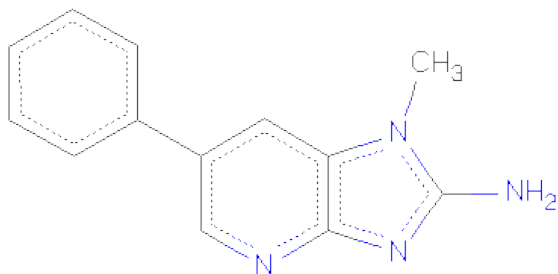
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	SER	-	EXPRESSION TAG	UNP P03372
A	537	SER	TYR	ENGINEERED	UNP P03372
B	297	SER	-	EXPRESSION TAG	UNP P03372
B	537	SER	TYR	ENGINEERED	UNP P03372

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	0	0
			95	60	20	15			
2	D	10	Total	C	N	O	0	0	0
			83	53	17	13			

- Molecule 3 is 2-AMINO-1-METHYL-6-PHENYLMIDAZO[4,5-B]PYRIDINE (three-letter code: PIQ) (formula: C<sub>13</sub>H<sub>12</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			17	13	4		
3	B	1	Total	C	N	0	0
			17	13	4		

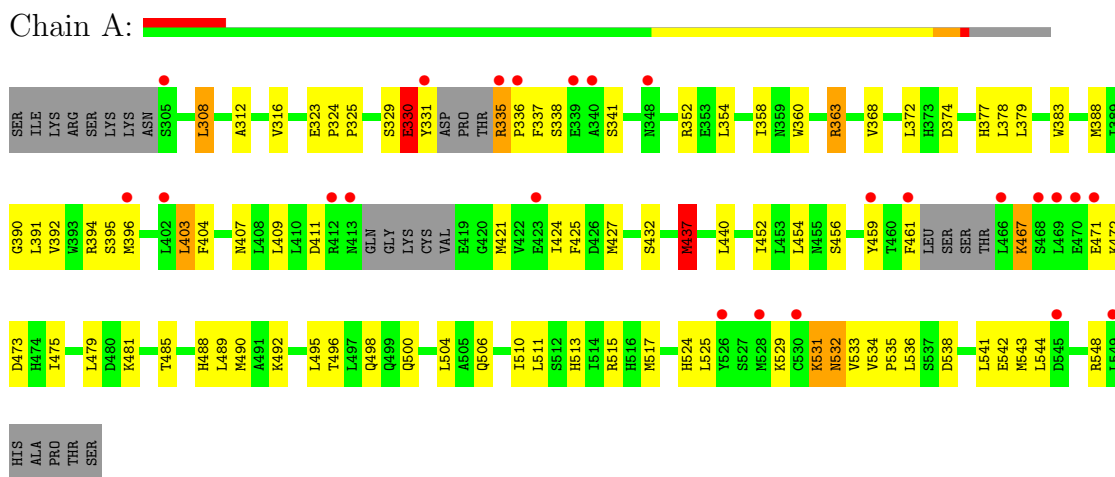
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	1	Total	O	0	0
			1	1		

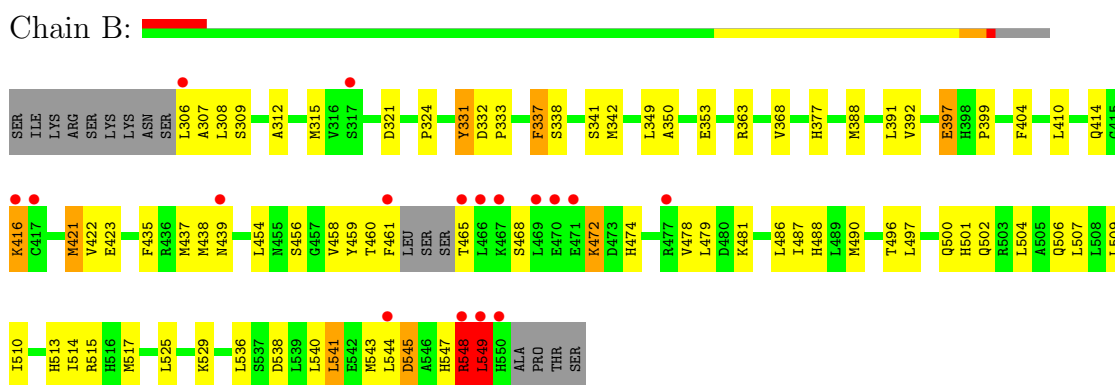
### 3 Residue-property plots

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.

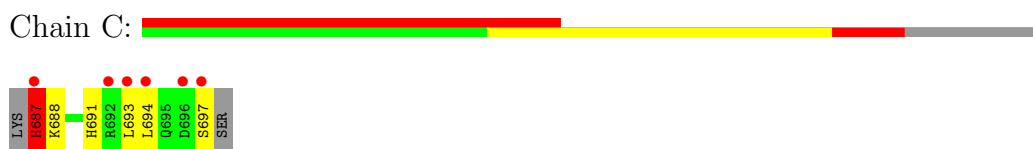
#### • Molecule 1: Estrogen receptor



#### • Molecule 1: Estrogen receptor

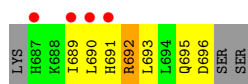


#### • Molecule 2: Nuclear receptor coactivator 2



#### • Molecule 2: Nuclear receptor coactivator 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.97Å 83.70Å 58.43Å 90.00° 108.70° 90.00°	Depositor
Resolution (Å)	11.96 – 2.30 11.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	88.5 (11.96-2.30) 88.5 (11.92-2.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.273 , 0.296 0.275 , 0.297	Depositor DCC
$R_{free}$ test set	1040 reflections (5.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.2	EDS
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 20137 reflections (0.010%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3997	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: PIQ

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	10/1878 (0.5%)	0.85	10/2536 (0.4%)
1	B	0.87	10/1995 (0.5%)	0.82	5/2696 (0.2%)
2	C	0.47	0/96	0.69	0/127
2	D	0.54	0/82	0.73	0/106
All	All	0.82	20/4051 (0.5%)	0.83	15/5465 (0.3%)

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
2	C	0	1
All	All	0	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	331	TYR	CB-CG	-9.13	1.38	1.51
1	B	331	TYR	CE2-CZ	-7.30	1.29	1.38
1	B	331	TYR	CG-CD1	-7.10	1.29	1.39
1	B	331	TYR	N-CA	-7.09	1.32	1.46
1	B	363	ARG	CZ-NH1	-6.85	1.24	1.33
1	A	337	PHE	CE1-CZ	-6.78	1.24	1.37
1	B	549	LEU	C-O	-6.57	1.10	1.23
1	A	331	TYR	CE1-CZ	6.35	1.46	1.38
1	A	337	PHE	CG-CD2	-6.28	1.29	1.38
1	B	337	PHE	CE1-CZ	-6.12	1.25	1.37
1	A	363	ARG	CZ-NH1	-5.86	1.25	1.33
1	A	337	PHE	CE2-CZ	-5.85	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	397	GLU	CG-CD	-5.85	1.43	1.51
1	A	548	ARG	CA-C	-5.84	1.37	1.52
1	B	548	ARG	CA-C	-5.67	1.38	1.52
1	A	337	PHE	CG-CD1	-5.38	1.30	1.38
1	A	330	GLU	CD-OE1	-5.17	1.20	1.25
1	A	531	LYS	CD-CE	-5.13	1.38	1.51
1	B	337	PHE	CG-CD2	-5.05	1.31	1.38
1	A	492	LYS	CD-CE	-5.01	1.38	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	ARG	NE-CZ-NH2	9.60	125.10	120.30
1	A	331	TYR	CB-CG-CD2	-8.98	115.61	121.00
1	A	363	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	A	421	MET	CG-SD-CE	-6.87	89.20	100.20
1	A	331	TYR	N-CA-C	6.53	128.62	111.00
1	B	437	MET	CG-SD-CE	-6.37	90.00	100.20
1	A	331	TYR	CG-CD1-CE1	-6.20	116.34	121.30
1	A	331	TYR	CB-CG-CD1	6.04	124.62	121.00
1	B	331	TYR	CG-CD2-CE2	5.93	126.05	121.30
1	B	421	MET	CG-SD-CE	-5.86	90.82	100.20
1	A	331	TYR	CD1-CE1-CZ	5.64	124.87	119.80
1	A	335	ARG	N-CA-CB	5.62	120.72	110.60
1	B	331	TYR	CA-CB-CG	-5.40	103.13	113.40
1	A	363	ARG	NH1-CZ-NH2	-5.12	113.76	119.40
1	A	437	MET	CG-SD-CE	-5.01	92.17	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	GLU	Peptide
2	C	687	HIS	Peptide

## 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	1840	0	1869	68	0
1	B	1941	0	1991	71	0
2	C	95	0	100	11	0
2	D	83	0	87	8	0
3	A	17	0	12	5	0
3	B	17	0	12	11	0
4	A	3	0	0	1	0
4	B	1	0	0	0	0
All	All	3997	0	4071	143	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 18.

All (143) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:421:MET:CE	3:B:1:PIQ:HM3	1.69	1.22
1:B:421:MET:HE3	3:B:1:PIQ:HM3	1.31	1.06
1:B:421:MET:HE1	3:B:1:PIQ:HM3	1.52	0.92
1:B:547:HIS:HB3	1:B:549:LEU:HD13	1.53	0.90
1:A:461:PHE:HB2	1:A:472:LYS:HE2	1.59	0.83
1:A:358:ILE:HD12	2:C:693:LEU:HD23	1.60	0.83
1:A:533:VAL:HG12	1:A:534:VAL:HG22	1.61	0.83
1:B:461:PHE:HB2	1:B:472:LYS:HE2	1.60	0.81
1:B:421:MET:HE3	3:B:1:PIQ:CM	2.12	0.79
1:A:391:LEU:HD22	3:A:1:PIQ:H3'	1.64	0.78
1:B:308:LEU:HA	1:B:481:LYS:HD2	1.67	0.76
1:A:358:ILE:CD1	2:C:693:LEU:HD23	2.17	0.75
1:A:335:ARG:CB	1:A:336:PRO:CD	2.65	0.74
1:A:388:MET:O	1:A:392:VAL:HG23	1.88	0.74
1:A:358:ILE:HG23	2:C:694:LEU:HD23	1.70	0.73
2:D:696:ASP:CG	2:D:696:ASP:CA	2.57	0.73
1:A:391:LEU:HD22	3:A:1:PIQ:C3'	2.17	0.72
1:B:461:PHE:HB2	1:B:472:LYS:CE	2.19	0.70
1:B:547:HIS:HB3	1:B:549:LEU:CD1	2.21	0.69
1:B:465:THR:N	1:B:468:SER:HG	1.90	0.69
1:B:421:MET:CE	3:B:1:PIQ:CM	2.61	0.69
1:B:435:PHE:CE1	1:B:510:ILE:HG21	2.27	0.68
1:A:383:TRP:CD1	1:A:543:MET:HE2	2.29	0.68
1:B:545:ASP:O	1:B:548:ARG:N	2.26	0.67
2:D:692:ARG:HG3	2:D:692:ARG:NH1	2.10	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:461:PHE:CB	1:B:472:LYS:HE2	2.25	0.67
1:A:525:LEU:HD13	3:A:1:PIQ:N3	2.10	0.67
1:A:531:LYS:HG2	1:A:533:VAL:HG23	1.78	0.66
1:A:533:VAL:HG12	1:A:534:VAL:CG2	2.25	0.65
1:A:391:LEU:CD2	3:A:1:PIQ:H3'	2.26	0.65
1:B:438:MET:O	1:B:439:ASN:HB3	1.95	0.65
2:D:692:ARG:HH11	2:D:692:ARG:HG3	1.62	0.64
1:B:547:HIS:O	1:B:549:LEU:HD12	1.98	0.64
1:A:383:TRP:CD1	1:A:543:MET:CE	2.81	0.63
1:A:377:HIS:HD2	1:A:461:PHE:CE1	2.17	0.62
1:B:306:LEU:HD12	1:B:307:ALA:H	1.64	0.62
1:A:513:HIS:HB2	1:B:459:TYR:CE2	2.35	0.62
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.80	0.62
1:B:331:TYR:CD2	1:B:332:ASP:N	2.68	0.62
1:A:461:PHE:CB	1:A:472:LYS:HE2	2.30	0.61
1:A:396:MET:HA	1:A:432[A]:SER:OG	2.01	0.60
1:B:377:HIS:NE2	1:B:460:THR:OG1	2.34	0.59
1:A:358:ILE:HG23	2:C:694:LEU:CD2	2.32	0.59
1:B:438:MET:HE2	1:B:507:LEU:HD21	1.84	0.58
1:A:403:LEU:HD12	1:A:409:LEU:HD13	1.85	0.58
1:B:506:GLN:O	1:B:510:ILE:HG13	2.03	0.58
1:B:331:TYR:OH	1:B:333:PRO:HA	2.03	0.57
2:C:687:HIS:CE1	2:C:688:LYS:HE3	2.39	0.57
1:B:416:LYS:NZ	1:B:416:LYS:HB2	2.19	0.57
1:B:421:MET:HE1	3:B:1:PIQ:CM	2.30	0.56
1:A:424:ILE:HA	1:A:427:MET:CE	2.35	0.56
1:B:461:PHE:CB	1:B:472:LYS:CE	2.83	0.56
1:A:513:HIS:HB2	1:B:459:TYR:CD2	2.40	0.56
1:A:335:ARG:CB	1:A:336:PRO:HD2	2.35	0.56
1:A:352:ARG:HD2	4:A:4:HOH:O	2.06	0.56
1:A:532:ASN:HD22	1:A:532:ASN:N	2.03	0.56
1:A:383:TRP:CG	1:A:543:MET:HE2	2.42	0.54
1:B:496:THR:O	1:B:500:GLN:HG3	2.06	0.54
1:B:547:HIS:CB	1:B:549:LEU:HD13	2.33	0.54
1:A:485:THR:O	1:A:489:LEU:HG	2.07	0.54
2:C:687:HIS:NE2	2:C:688:LYS:HE3	2.22	0.54
1:A:329:SER:OG	1:A:330:GLU:N	2.41	0.53
1:B:331:TYR:C	1:B:331:TYR:CD2	2.71	0.53
1:A:535:PRO:O	1:A:536:LEU:HD23	2.08	0.53
1:B:525:LEU:HD23	1:B:544:LEU:HD13	1.92	0.52
1:B:337:PHE:CD2	1:B:342[A]:MET:HE2	2.45	0.52
1:A:338:SER:OG	1:A:341:SER:HB3	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:379:LEU:HD12	2:C:694:LEU:HD21	1.91	0.52
1:A:379:LEU:CD1	2:C:694:LEU:HD21	2.40	0.51
1:B:538:ASP:HB3	2:D:689:ILE:HD11	1.93	0.50
1:A:531:LYS:HE2	1:A:533:VAL:HG21	1.94	0.50
1:B:391:LEU:HB2	3:B:1:PIQ:H3'	1.93	0.49
1:A:456:SER:HA	1:A:515:ARG:NH2	2.28	0.49
1:A:424:ILE:HA	1:A:427:MET:HE3	1.95	0.49
1:B:350:ALA:HB2	3:B:1:PIQ:H5	1.95	0.48
1:B:547:HIS:O	1:B:549:LEU:N	2.46	0.48
1:A:374:ASP:O	1:A:378:LEU:HG	2.14	0.48
1:A:506:GLN:O	1:A:510:ILE:HG13	2.14	0.48
1:A:396:MET:HE1	1:A:440:LEU:HB3	1.94	0.47
1:A:329:SER:HB3	1:A:407:ASN:OD1	2.14	0.47
1:B:536:LEU:HB2	1:B:541:LEU:HD13	1.96	0.47
1:A:395:SER:O	1:A:396:MET:C	2.53	0.47
1:A:471:GLU:O	1:A:475:ILE:HG13	2.13	0.47
1:B:454:LEU:HB2	1:B:479:LEU:HD21	1.97	0.47
1:B:353:GLU:OE1	3:B:1:PIQ:C5'	2.63	0.47
1:A:391:LEU:HD13	1:A:404:PHE:HA	1.97	0.47
1:A:496:THR:O	1:A:500:GLN:HG3	2.15	0.46
1:B:486:LEU:O	1:B:490:MET:HG3	2.16	0.46
1:A:424:ILE:HA	1:A:427:MET:HE2	1.98	0.46
1:B:388:MET:O	1:B:392:VAL:HG23	2.16	0.46
1:B:350:ALA:HB2	3:B:1:PIQ:H6'	1.98	0.45
1:A:538:ASP:O	1:A:542:GLU:HG3	2.16	0.45
1:B:416:LYS:HA	1:B:416:LYS:HE3	1.98	0.44
1:A:504:LEU:HD23	1:B:504:LEU:HD23	1.97	0.44
1:B:501:HIS:CD2	1:B:501:HIS:C	2.90	0.44
1:B:487:ILE:O	1:B:488:HIS:C	2.56	0.44
2:D:692:ARG:HH11	2:D:692:ARG:CG	2.26	0.44
1:A:312:ALA:HB1	1:A:488:HIS:CG	2.53	0.44
1:B:541:LEU:HD12	1:B:541:LEU:HA	1.84	0.44
1:A:525:LEU:HG	1:A:544:LEU:HD22	1.99	0.43
1:B:349:LEU:HD21	1:B:404:PHE:O	2.18	0.43
1:B:353:GLU:OE1	3:B:1:PIQ:H5'	2.18	0.43
1:B:410:LEU:HA	1:B:414:GLN:OE1	2.18	0.43
1:A:524:HIS:ND1	3:A:1:PIQ:N	2.65	0.43
1:B:397:GLU:C	1:B:399:PRO:HD3	2.39	0.43
1:B:474:HIS:O	1:B:478:VAL:HG23	2.18	0.43
1:B:547:HIS:C	1:B:549:LEU:N	2.72	0.43
1:A:358:ILE:CD1	2:C:693:LEU:CD2	2.93	0.43
1:B:332:ASP:HA	1:B:333:PRO:HD2	1.93	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:467:LYS:HD2	1:A:467:LYS:HA	1.57	0.43
1:A:459:TYR:CD2	1:B:513:HIS:HB2	2.54	0.43
1:A:427:MET:CE	1:A:517:MET:HG2	2.48	0.42
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.82	0.42
2:D:691:HIS:CD2	2:D:695:GLN:HE21	2.37	0.42
1:B:509:LEU:HA	1:B:509:LEU:HD23	1.80	0.42
1:B:547:HIS:O	1:B:549:LEU:CD1	2.66	0.42
1:A:358:ILE:CG2	2:C:694:LEU:HD23	2.46	0.42
1:B:338:SER:OG	1:B:341:SER:HB3	2.18	0.42
1:A:490:MET:HB3	1:A:495:LEU:HD22	2.02	0.42
1:B:438:MET:CE	1:B:507:LEU:CD2	2.97	0.42
1:A:454:LEU:HB2	1:A:479:LEU:HD21	2.02	0.42
1:B:540[A]:LEU:HD23	1:B:540[A]:LEU:HA	1.76	0.42
1:A:452:ILE:HD11	1:A:511:LEU:HD22	2.02	0.42
1:A:308:LEU:HD23	1:A:308:LEU:N	2.35	0.42
1:A:323:GLU:HA	1:A:324:PRO:HD2	1.85	0.42
1:B:312:ALA:O	1:B:315:MET:HB3	2.20	0.41
1:B:456:SER:HA	1:B:515:ARG:NH2	2.35	0.41
1:A:379:LEU:HD23	1:A:379:LEU:HA	1.91	0.41
1:B:536:LEU:N	1:B:536:LEU:HD12	2.36	0.41
1:A:390:GLY:O	1:A:394:ARG:HG3	2.21	0.41
1:A:437:MET:HG3	1:A:437:MET:O	2.20	0.41
1:B:514:ILE:HA	1:B:517:MET:HE2	2.03	0.41
2:C:688:LYS:O	2:C:691:HIS:HB3	2.21	0.41
1:B:501:HIS:CD2	1:B:502:GLN:N	2.89	0.41
1:A:324:PRO:HA	1:A:325:PRO:HD3	1.93	0.41
1:B:543:MET:SD	2:D:690:LEU:HD22	2.61	0.41
1:B:548:ARG:CZ	1:B:548:ARG:HB2	2.51	0.41
2:D:689:ILE:O	2:D:693:LEU:HG	2.21	0.41
1:A:459:TYR:CE2	1:B:513:HIS:HB2	2.56	0.41
1:A:377:HIS:CD2	1:A:461:PHE:CE1	3.05	0.41
1:B:438:MET:CE	1:B:507:LEU:HD21	2.49	0.40
1:B:422:VAL:HG13	1:B:423:GLU:N	2.36	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	227/258 (88%)	220 (97%)	7 (3%)	0	100	100
1	B	244/258 (95%)	231 (95%)	12 (5%)	1 (0%)	43	52
2	C	9/13 (69%)	9 (100%)	0	0	100	100
2	D	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
All	All	488/542 (90%)	467 (96%)	20 (4%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	548	ARG

### 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	204/233 (88%)	187 (92%)	17 (8%)	16	19
1	B	219/233 (94%)	206 (94%)	13 (6%)	28	35
2	C	11/13 (85%)	9 (82%)	2 (18%)	2	2
2	D	8/13 (62%)	7 (88%)	1 (12%)	7	7
All	All	442/492 (90%)	409 (92%)	33 (8%)	19	23

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	LEU
1	A	330	GLU
1	A	360	TRP
1	A	363	ARG
1	A	368	VAL
1	A	372	LEU
1	A	403	LEU
1	A	411	ASP

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Mol	Chain	Res	Type
1	A	425	PHE
1	A	437	MET
1	A	467	LYS
1	A	473	ASP
1	A	481	LYS
1	A	498	GLN
1	A	529	LYS
1	A	532	ASN
1	A	541	LEU
1	B	309	SER
1	B	321	ASP
1	B	324	PRO
1	B	368	VAL
1	B	416	LYS
1	B	458	VAL
1	B	472	LYS
1	B	497	LEU
1	B	529	LYS
1	B	541	LEU
1	B	545	ASP
1	B	548	ARG
1	B	549	LEU
2	C	687	HIS
2	C	697	SER
2	D	692	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	HIS
1	A	532	ASN
1	B	513	HIS
2	C	687	HIS
2	D	691	HIS
2	D	695	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	PIQ	A	1	-	19,19,19	1.71	4 (21%)	25,27,27	1.78	4 (16%)
3	PIQ	B	1	-	19,19,19	1.53	3 (15%)	25,27,27	1.66	6 (24%)

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	PIQ	A	1	-	-	0/4/4/4	0/1/3/3
3	PIQ	B	1	-	-	0/4/4/4	0/1/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	PIQ	C7A-N1	-4.58	1.33	1.39
3	A	1	PIQ	C7A-N1	-4.24	1.33	1.39
3	A	1	PIQ	C2-N1	-3.91	1.32	1.35
3	A	1	PIQ	C1'-C6	-3.13	1.40	1.49
3	B	1	PIQ	C1'-C6	-3.01	1.40	1.49
3	B	1	PIQ	C2-N1	-2.68	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	PIQ	C3A-N3	-2.56	1.33	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	PIQ	C6-C7-C7A	-5.39	117.66	122.10
3	B	1	PIQ	C6-C7-C7A	-3.75	119.01	122.10
3	A	1	PIQ	C5-N4-C3A	3.59	120.88	116.85
3	A	1	PIQ	C6-C5-N4	-3.45	120.84	125.60
3	B	1	PIQ	C5-N4-C3A	3.38	120.64	116.85
3	B	1	PIQ	N4-C3A-N3	2.88	133.68	125.81
3	B	1	PIQ	C7A-C3A-N4	-2.71	119.42	125.33
3	B	1	PIQ	C6-C5-N4	-2.47	122.19	125.60
3	A	1	PIQ	N4-C3A-N3	2.19	131.80	125.81
3	B	1	PIQ	C7A-C3A-N3	-2.10	106.90	109.26

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, 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	233/258 (90%)	0.62	24 (10%) 7 11	11, 29, 57, 75	4 (1%)
1	B	242/258 (93%)	0.48	17 (7%) 16 23	7, 30, 55, 75	0
2	C	11/13 (84%)	3.09	6 (54%) 0 0	28, 39, 61, 72	0
2	D	10/13 (76%)	1.68	4 (40%) 1 1	18, 35, 49, 57	0
All	All	496/542 (91%)	0.63	51 (10%) 7 11	7, 30, 57, 75	4 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	697	SER	6.7
2	C	696	ASP	6.2
1	B	550	HIS	6.0
1	A	469	LEU	6.0
1	A	335	ARG	5.9
1	B	466	LEU	5.8
2	C	694	LEU	5.7
1	B	549	LEU	5.3
1	A	466	LEU	5.3
2	C	687	HIS	5.2
1	B	465	THR	5.2
1	B	469	LEU	5.0
1	A	331	TYR	4.8
1	B	417	CYS	4.6
2	D	687	HIS	4.6
1	A	549	LEU	4.1
1	A	413	ASN	4.1
2	C	693	LEU	3.8
1	A	528	MET	3.6
1	A	530	CYS	3.3
2	D	690	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	396	MET	3.2
1	B	306	LEU	3.1
1	B	461	PHE	3.1
1	B	471	GLU	3.0
1	A	459	TYR	3.0
1	A	461	PHE	2.9
1	A	526	TYR	2.9
1	A	305	SER	2.9
1	A	412	ARG	2.8
1	A	468	SER	2.8
1	B	477	ARG	2.8
1	A	336	PRO	2.8
1	B	416	LYS	2.7
1	A	423	GLU	2.6
1	B	439	ASN	2.6
1	B	470	GLU	2.6
1	A	470	GLU	2.6
1	B	467	LYS	2.5
1	B	548	ARG	2.5
2	D	689	ILE	2.5
1	B	317	SER	2.4
1	A	545	ASP	2.3
1	A	340	ALA	2.3
1	A	339	GLU	2.3
2	C	692	ARG	2.2
1	A	348	ASN	2.2
1	B	544	LEU	2.2
2	D	691	HIS	2.1
1	A	402	LEU	2.1
1	A	471	GLU	2.1

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

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

## 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PIQ	B	1	17/17	0.17	1.16	18,40,67,77	0
3	PIQ	A	1	17/17	0.17	0.98	19,47,60,61	0

## 6.5 Other polymers

There are no such residues in this entry.