Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 11:47 AM EDT

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 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

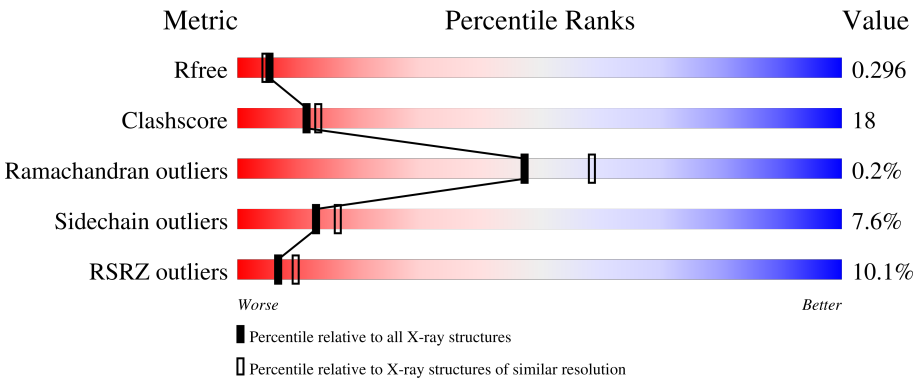
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	258	9%, 56%, 31%, • •, 10%
1	B	258	7%, 63%, 27%, • •, 6%
2	C	13	46%, 38%, 38%, 8%, 15%
2	D	13	23%, 23%, 46%, 8%, 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PIQ	B	1	-	-	X	-

2 Entry composition (i)

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

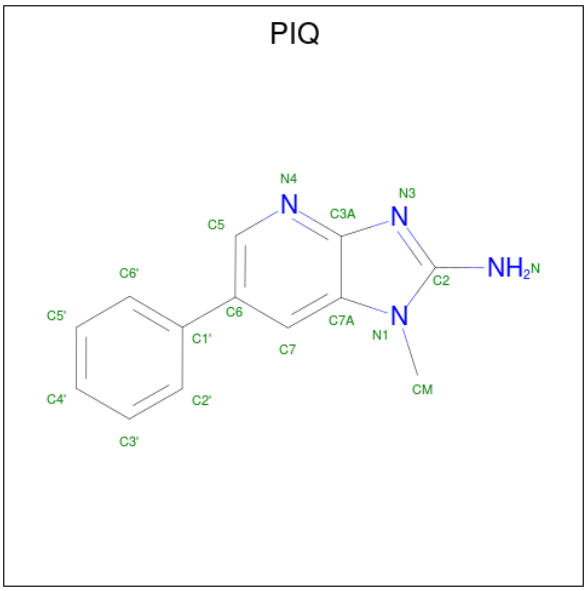
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	SER	-	expression tag	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372
B	297	SER	-	expression tag	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

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

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

- Molecule 3 is 2-AMINO-1-METHYL-6-PHENYLIMIDAZO[4,5-B]PYRIDINE (three-letter code: PIQ) (formula: $C_{13}H_{12}N_4$).



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

- Molecule 4 is water.

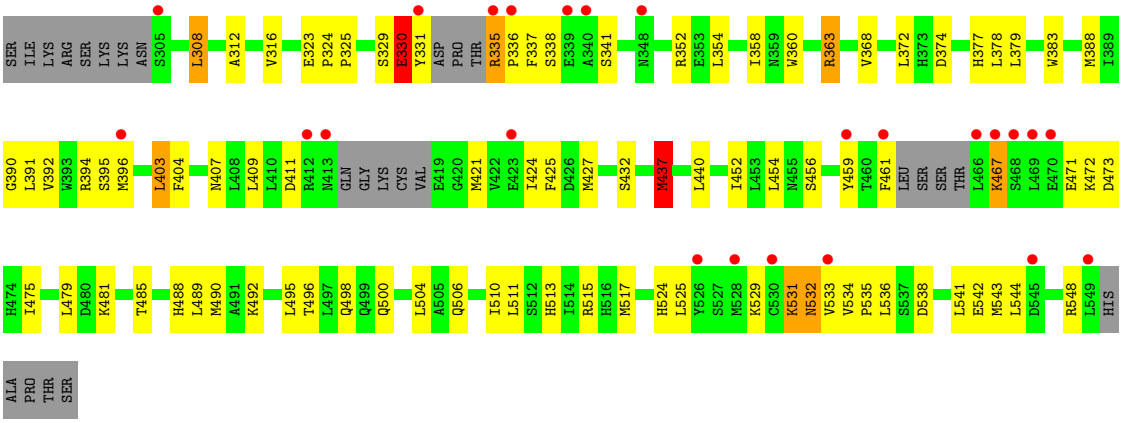
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

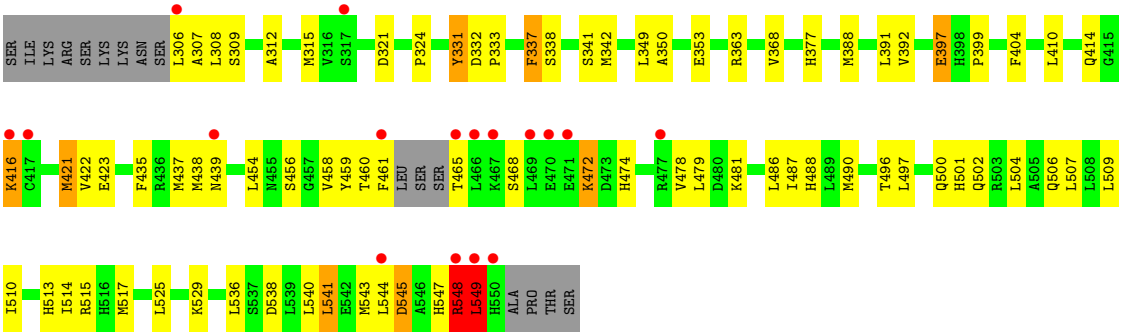
• Molecule 1: Estrogen receptor

Chain A:



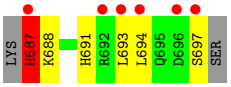
• Molecule 1: Estrogen receptor

Chain B:



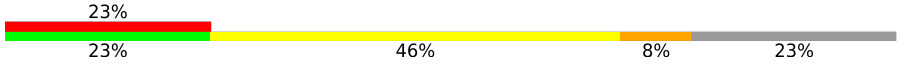
• Molecule 2: Nuclear receptor coactivator 2

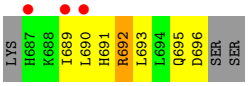
Chain C:



• Molecule 2: Nuclear receptor coactivator 2

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.57 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.273 , 0.296 0.273 , 0.296	Depositor DCC
R_{free} test set	1040 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3997	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 5.90% 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, 0.333 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: 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(^{o})	Ideal(^{o})
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 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	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

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 18.

All (143) 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: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:CA	2:D:696:ASP:CG	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:NH1	2:D:692:ARG:HG3	2.10	0.67
1:A:525:LEU:HD13	3:A:1:PIQ:N3	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:PHE:CB	1:B:472:LYS:HE2	2.25	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:HG3	2:D:692:ARG:HH11	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:316:VAL:HG21	1:A:489:LEU:HD21	1.80	0.62
1:A:513:HIS:HB2	1:B:459:TYR:CE2	2.35	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:A:403:LEU:HD12	1:A:409:LEU:HD13	1.85	0.58
1:B:438:MET:HE2	1:B:507:LEU:HD21	1.84	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
1:B:416:LYS:NZ	1:B:416:LYS:HB2	2.19	0.57
2:C:687:HIS:CE1	2:C:688:LYS:HE3	2.39	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:A:513:HIS:HB2	1:B:459:TYR:CD2	2.40	0.56
1:B:461:PHE:CB	1:B:472:LYS:CE	2.83	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:N	1:A:532:ASN:HD22	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:A:485:THR:O	1:A:489:LEU:HG	2.07	0.54
1:B:547:HIS:CB	1:B:549:LEU:HD13	2.33	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:CD2	1:B:331:TYR:C	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	Interatomic distance (Å)	Clash overlap (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:329:SER:HB3	1:A:407:ASN:OD1	2.14	0.47
1:A:396:MET:HE1	1:A:440:LEU:HB3	1.94	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:HE3	1:B:416:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ASP:HA	1:B:333:PRO:HD2	1.93	0.43
1:A:467:LYS:HA	1:A:467:LYS:HD2	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:HD23	1:B:509:LEU:HA	1.80	0.42
1:A:358:ILE:CG2	2:C:694:LEU:HD23	2.46	0.42
1:B:547:HIS:O	1:B:549:LEU:CD1	2.66	0.42
1:A:490:MET:HB3	1:A:495:LEU:HD22	2.02	0.42
1:B:338:SER:OG	1:B:341:SER:HB3	2.18	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:HA	1:B:540[A]:LEU:HD23	1.76	0.42
1:A:308:LEU:HD23	1:A:308:LEU:N	2.35	0.42
1:A:452:ILE:HD11	1:A:511:LEU:HD22	2.02	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:A:390:GLY:O	1:A:394:ARG:HG3	2.21	0.41
1:A:437:MET:O	1:A:437:MET:HG3	2.20	0.41
1:B:536:LEU:HD12	1:B:536:LEU:N	2.36	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:A:324:PRO:HA	1:A:325:PRO:HD3	1.93	0.41
1:B:501:HIS:CD2	1:B:502:GLN:N	2.89	0.41
1:B:543:MET:SD	2:D:690:LEU:HD22	2.61	0.41
1:A:459:TYR:CE2	1:B:513:HIS:HB2	2.56	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:377:HIS:CD2	1:A:461:PHE:CE1	3.05	0.41
1:B:422:VAL:HG13	1:B:423:GLU:N	2.36	0.40
1:B:438:MET:CE	1:B:507:LEU:HD21	2.49	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	227/258 (88%)	220 (97%)	7 (3%)	0	100	100
1	B	244/258 (95%)	231 (95%)	12 (5%)	1 (0%)	34	42
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%)	47	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	548	ARG

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	204/233 (88%)	187 (92%)	17 (8%)	11	14
1	B	219/233 (94%)	206 (94%)	13 (6%)	19	27
2	C	11/13 (85%)	9 (82%)	2 (18%)	1	1
2	D	8/13 (62%)	7 (88%)	1 (12%)	4	5
All	All	442/492 (90%)	409 (92%)	33 (8%)	13	17

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
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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	-	15,19,19	0.99	0	10,27,27	1.49	2 (20%)
3	PIQ	B	1	-	15,19,19	1.04	1 (6%)	10,27,27	1.12	1 (10%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	PIQ	C5-N4	2.69	1.33	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	PIQ	C6-C5-N4	-3.10	120.84	125.05
3	A	1	PIQ	C6-C7-C7A	-2.98	117.66	120.86
3	B	1	PIQ	C6-C5-N4	-2.10	122.19	125.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	PIQ	5	0
3	B	1	PIQ	11	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, 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	233/258 (90%)	0.48	24 (10%)	6	9	11, 29, 57, 75	4 (1%)
1	B	242/258 (93%)	0.34	17 (7%)	16	21	7, 30, 55, 75	0
2	C	11/13 (84%)	3.22	6 (54%)	0	0	28, 39, 61, 72	0
2	D	10/13 (76%)	1.56	3 (30%)	0	0	18, 35, 49, 57	0
All	All	496/542 (91%)	0.49	50 (10%)	7	9	7, 30, 57, 75	4 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	697	SER	8.1
1	B	550	HIS	6.9
1	A	469	LEU	6.4
1	A	335	ARG	5.9
2	C	696	ASP	5.8
2	C	694	LEU	5.8
2	C	687	HIS	5.6
1	B	466	LEU	5.4
1	A	466	LEU	5.3
1	A	331	TYR	5.0
2	D	687	HIS	4.8
1	B	465	THR	4.4
1	B	549	LEU	4.2
1	A	549	LEU	4.2
1	B	417	CYS	4.1
1	A	413	ASN	4.0
1	B	469	LEU	4.0
2	C	693	LEU	3.7
1	A	528	MET	3.3
1	A	423	GLU	3.3
1	A	396	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	306	LEU	3.2
1	A	305	SER	3.1
1	B	416	LYS	3.1
2	D	690	LEU	3.0
1	A	412	ARG	3.0
1	A	459	TYR	3.0
1	A	461	PHE	2.9
1	B	471	GLU	2.9
1	A	530	CYS	2.9
1	A	336	PRO	2.9
1	B	461	PHE	2.8
1	A	470	GLU	2.6
1	A	340	ALA	2.6
1	B	477	ARG	2.5
2	D	689	ILE	2.4
1	A	468	SER	2.4
1	A	526	TYR	2.3
1	B	544	LEU	2.3
1	B	470	GLU	2.3
2	C	692	ARG	2.2
1	B	467	LYS	2.2
1	B	548	ARG	2.2
1	A	348	ASN	2.2
1	A	339	GLU	2.2
1	B	439	ASN	2.2
1	B	317	SER	2.1
1	A	533	VAL	2.1
1	A	545	ASP	2.0
1	A	467	LYS	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 monosaccharides 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. 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PIQ	B	1	17/17	0.88	0.20	18,40,67,77	0
3	PIQ	A	1	17/17	0.91	0.20	19,47,60,61	0

6.5 Other polymers (i)

There are no such residues in this entry.