



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:07 pm GMT

PDB ID : 1TFC
Title : CRYSTAL STRUCTURE OF THE LIGAND-BINDING DOMAIN OF THE ESTROGEN-RELATED RECEPTOR GAMMA IN COMPLEX WITH A STEROID RECEPTOR COACTIVATOR-1 PEPTIDE
Authors : Greschik, H.; Flaig, R.; Renaud, J.P.; Moras, D.
Deposited on : 2004-05-27
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 ⓘ symbol.

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

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

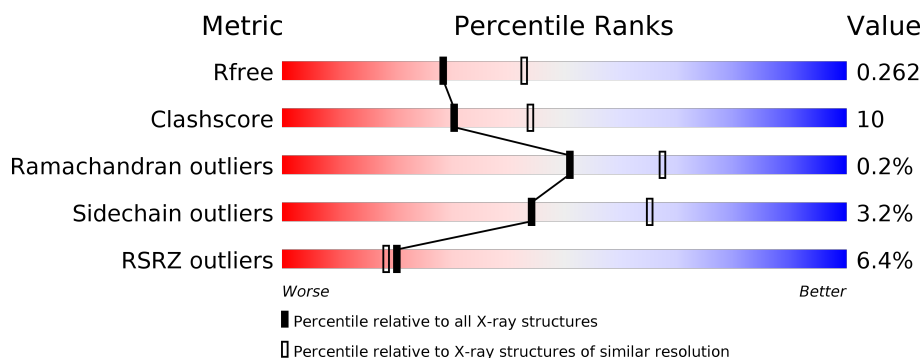
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	251	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>• 10%</div> </div> </div>
1	B	251	<div> <div>8%</div> <div> <div></div> <div>61%</div> <div>27%</div> <div>• 10%</div> </div> </div>
2	C	15	<div> <div>13%</div> <div> <div></div> <div>60%</div> <div>13%</div> <div>27%</div> </div> </div>
2	D	15	<div> <div>20%</div> <div> <div></div> <div>33%</div> <div>20%</div> <div>13%</div> <div>33%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3739 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-related receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1779	1142	288	337	12			
1	B	225	Total	C	N	O	S	0	0	0
			1758	1126	286	334	12			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	MET	-	EXPRESSION TAG	UNP P62508
A	209	GLY	-	EXPRESSION TAG	UNP P62508
A	210	SER	-	EXPRESSION TAG	UNP P62508
A	211	SER	-	EXPRESSION TAG	UNP P62508
A	212	HIS	-	EXPRESSION TAG	UNP P62508
A	213	HIS	-	EXPRESSION TAG	UNP P62508
A	214	HIS	-	EXPRESSION TAG	UNP P62508
A	215	HIS	-	EXPRESSION TAG	UNP P62508
A	216	HIS	-	EXPRESSION TAG	UNP P62508
A	217	HIS	-	EXPRESSION TAG	UNP P62508
A	218	SER	-	EXPRESSION TAG	UNP P62508
A	219	SER	-	EXPRESSION TAG	UNP P62508
A	220	GLY	-	EXPRESSION TAG	UNP P62508
A	221	LEU	-	EXPRESSION TAG	UNP P62508
A	222	VAL	-	EXPRESSION TAG	UNP P62508
A	223	PRO	-	EXPRESSION TAG	UNP P62508
A	224	ARG	-	EXPRESSION TAG	UNP P62508
A	225	GLY	-	EXPRESSION TAG	UNP P62508
A	226	SER	-	EXPRESSION TAG	UNP P62508
A	227	HIS	-	EXPRESSION TAG	UNP P62508
A	228	MET	-	EXPRESSION TAG	UNP P62508
B	208	MET	-	EXPRESSION TAG	UNP P62508
B	209	GLY	-	EXPRESSION TAG	UNP P62508
B	210	SER	-	EXPRESSION TAG	UNP P62508
B	211	SER	-	EXPRESSION TAG	UNP P62508

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Chain	Residue	Modelled	Actual	Comment	Reference
B	212	HIS	-	EXPRESSION TAG	UNP P62508
B	213	HIS	-	EXPRESSION TAG	UNP P62508
B	214	HIS	-	EXPRESSION TAG	UNP P62508
B	215	HIS	-	EXPRESSION TAG	UNP P62508
B	216	HIS	-	EXPRESSION TAG	UNP P62508
B	217	HIS	-	EXPRESSION TAG	UNP P62508
B	218	SER	-	EXPRESSION TAG	UNP P62508
B	219	SER	-	EXPRESSION TAG	UNP P62508
B	220	GLY	-	EXPRESSION TAG	UNP P62508
B	221	LEU	-	EXPRESSION TAG	UNP P62508
B	222	VAL	-	EXPRESSION TAG	UNP P62508
B	223	PRO	-	EXPRESSION TAG	UNP P62508
B	224	ARG	-	EXPRESSION TAG	UNP P62508
B	225	GLY	-	EXPRESSION TAG	UNP P62508
B	226	SER	-	EXPRESSION TAG	UNP P62508
B	227	HIS	-	EXPRESSION TAG	UNP P62508
B	228	MET	-	EXPRESSION TAG	UNP P62508

- Molecule 2 is a protein called steroid receptor coactivator-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	0	0
			81	52	17	12			
2	D	10	Total	C	N	O	0	0	0
			81	52	16	13			

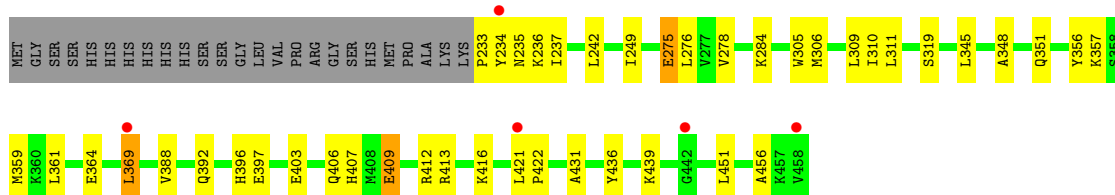
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	18	Total	O	0	0
			18	18		

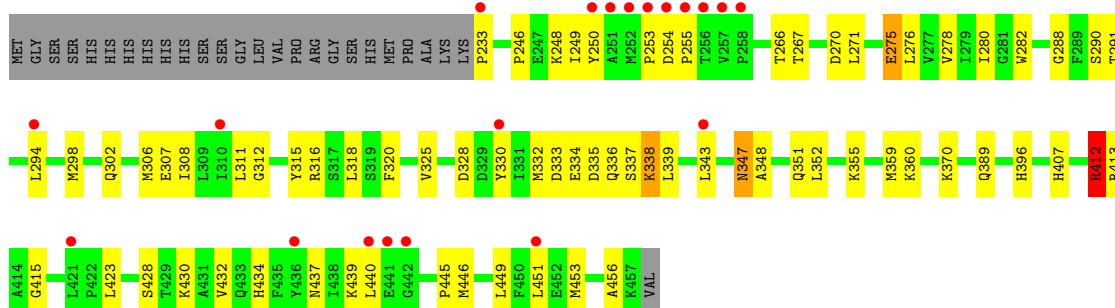
3 Residue-property plots

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

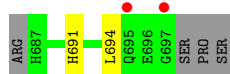
- Molecule 1: Estrogen-related receptor gamma



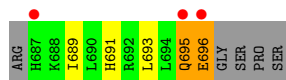
- Molecule 1: Estrogen-related receptor gamma



- Molecule 2: steroid receptor coactivator-1



- Molecule 2: steroid receptor coactivator-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	83.48Å 83.48Å 239.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.32 – 2.40 29.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.4 (24.32-2.40) 99.9 (29.59-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.33 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.258 0.248 , 0.262	Depositor DCC
R_{free} test set	1724 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.815	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3739	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.39	0/1810	0.59	1/2450 (0.0%)
1	B	0.37	0/1787	0.59	2/2420 (0.1%)
2	C	0.37	0/81	0.50	0/108
2	D	0.42	0/81	0.53	0/108
All	All	0.38	0/3759	0.59	3/5086 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	PRO	N-CA-CB	5.76	110.21	103.30
1	B	233	PRO	N-CA-CB	5.60	110.02	103.30
1	B	412	ARG	NE-CZ-NH2	-5.60	117.50	120.30

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	1779	0	1800	26	0
1	B	1758	0	1767	52	0
2	C	81	0	80	2	0
2	D	81	0	81	4	0
3	A	22	0	0	2	0
3	B	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3739	0	3728	78	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 10.

All (78) 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:343:LEU:O	1:B:347:ASN:HB2	1.83	0.79
1:B:439:LYS:HG3	1:B:451:LEU:CD2	2.15	0.77
1:B:298:MET:O	1:B:302:GLN:HG3	1.86	0.76
1:B:335:ASP:O	1:B:339:LEU:HG	1.88	0.72
1:B:348:ALA:O	1:B:351:GLN:HB2	1.90	0.72
1:B:334:GLU:O	1:B:338:LYS:HG2	1.97	0.64
1:B:439:LYS:HG3	1:B:451:LEU:HD22	1.79	0.63
1:A:249:ILE:HD11	1:A:278:VAL:HG21	1.80	0.63
1:A:412:ARG:HG2	1:B:396:HIS:CE1	2.32	0.63
1:B:253:PRO:HG3	1:B:330:TYR:CD1	2.34	0.62
1:A:359:MET:HE3	1:A:416:LYS:HB3	1.82	0.62
1:A:275:GLU:HB3	1:A:309:LEU:HD21	1.83	0.60
1:B:249:ILE:CG2	1:B:250:TYR:N	2.65	0.60
1:B:288:GLY:O	1:B:291:THR:HB	2.03	0.58
1:B:333:ASP:OD1	1:B:336:GLN:HG3	2.04	0.57
1:A:403:GLU:OE1	1:A:413:ARG:HD3	2.04	0.57
1:B:246:PRO:HB3	1:B:278:VAL:CG1	2.35	0.56
1:B:253:PRO:HG3	1:B:330:TYR:HD1	1.69	0.55
1:A:242:LEU:HD11	1:A:364:GLU:HG3	1.88	0.55
1:A:235:ASN:OD1	1:A:237:ILE:HB	2.06	0.55
1:A:234:TYR:HE1	1:A:406:GLN:OE1	1.91	0.54
1:B:307:GLU:HG2	1:B:428:SER:CB	2.38	0.54
1:B:312:GLY:O	1:B:316:ARG:HG3	2.08	0.54
1:B:294:LEU:O	1:B:298:MET:HG3	2.07	0.53
1:B:267:THR:HG21	1:B:330:TYR:CE1	2.43	0.53
1:B:332:MET:CE	1:B:337:SER:HA	2.39	0.53
1:A:407:HIS:HA	1:A:409:GLU:OE2	2.08	0.53
1:B:282:TRP:CH2	1:B:370:LYS:HG2	2.43	0.52
1:B:249:ILE:HG22	1:B:250:TYR:N	2.24	0.52
1:B:453:MET:O	1:B:456:ALA:HB3	2.08	0.52
1:A:234:TYR:N	1:A:234:TYR:CD2	2.70	0.51
1:B:270:ASP:C	1:B:270:ASP:OD1	2.49	0.50
1:B:248:LYS:HD3	1:B:328:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD21	1:A:305:TRP:CE3	2.47	0.49
1:B:275:GLU:O	1:B:278:VAL:HB	2.12	0.49
1:B:446:MET:HB2	1:B:451:LEU:HG	1.95	0.49
1:B:359:MET:O	1:B:360:LYS:HB2	2.13	0.49
1:B:266:THR:OG1	1:B:445:PRO:HD2	2.13	0.48
2:D:693:LEU:HA	2:D:696:GLU:OE1	2.13	0.48
1:B:246:PRO:HB3	1:B:278:VAL:HG13	1.95	0.48
1:B:449:LEU:HD13	2:D:689:ILE:CG2	2.44	0.47
1:A:388:VAL:O	1:A:392:GLN:HG3	2.13	0.47
1:B:276:LEU:O	1:B:280:ILE:HG13	2.14	0.47
1:A:236:LYS:HG3	3:A:31:HOH:O	2.13	0.47
1:A:436:TYR:O	1:A:439:LYS:HB3	2.14	0.47
1:B:343:LEU:HG	1:B:343:LEU:O	2.13	0.47
1:B:249:ILE:HG22	1:B:271:LEU:HD11	1.96	0.47
1:A:356:TYR:CD1	1:A:361:LEU:HD22	2.49	0.47
1:B:315:TYR:O	1:B:318:LEU:HG	2.15	0.46
1:A:345:LEU:HD11	1:A:431:ALA:HB2	1.97	0.46
1:B:434:HIS:O	1:B:437:ASN:HB2	2.15	0.46
2:D:691:HIS:O	2:D:695:GLN:HB2	2.15	0.46
1:A:348:ALA:O	1:A:351:GLN:HB2	2.15	0.46
1:B:320:PHE:CE1	1:B:325:VAL:HG21	2.50	0.46
1:A:356:TYR:CG	1:A:361:LEU:HD22	2.51	0.46
1:B:307:GLU:HG2	1:B:428:SER:OG	2.16	0.46
1:B:430:LYS:HE2	1:B:430:LYS:HB2	1.67	0.45
1:A:284:LYS:NZ	2:C:694:LEU:O	2.48	0.45
1:A:306:MET:O	1:A:310:ILE:HG13	2.16	0.45
1:B:338:LYS:HB3	1:B:338:LYS:HE3	1.82	0.44
1:B:355:LYS:O	1:B:359:MET:HG3	2.17	0.44
1:A:396:HIS:CE1	1:B:415:GLY:HA3	2.53	0.44
1:B:306:MET:HG2	1:B:432:VAL:HG23	1.99	0.43
1:A:397:GLU:HG3	1:B:412:ARG:NH2	2.33	0.43
1:A:421:LEU:N	1:A:422:PRO:CD	2.82	0.43
1:B:407:HIS:CG	1:B:413:ARG:HD3	2.54	0.42
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.89	0.42
1:B:352:LEU:HD23	1:B:423:LEU:HD23	2.02	0.42
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.85	0.42
1:B:254:ASP:OD1	1:B:255:PRO:HD2	2.20	0.41
1:B:311:LEU:HA	1:B:311:LEU:HD12	1.76	0.41
1:B:428:SER:O	1:B:432:VAL:HG23	2.20	0.41
1:B:440:LEU:HD23	1:B:440:LEU:HA	1.97	0.41
2:C:691:HIS:CD2	2:C:691:HIS:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ILE:HD12	2:D:693:LEU:HD12	2.02	0.41
1:B:254:ASP:HA	1:B:255:PRO:HD3	1.86	0.41
1:B:308:ILE:HG23	1:B:370:LYS:HD2	2.03	0.41
1:A:357:LYS:NZ	3:A:40:HOH:O	2.53	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	224/251 (89%)	216 (96%)	7 (3%)	1 (0%)	38	54
1	B	223/251 (89%)	215 (96%)	8 (4%)	0	100	100
2	C	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	D	8/15 (53%)	7 (88%)	1 (12%)	0	100	100
All	All	464/532 (87%)	446 (96%)	17 (4%)	1 (0%)	51	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	ALA

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	195/221 (88%)	190 (97%)	5 (3%)	51	72
1	B	191/221 (86%)	185 (97%)	6 (3%)	45	66
2	C	7/14 (50%)	7 (100%)	0	100	100
2	D	8/14 (57%)	6 (75%)	2 (25%)	1	0
All	All	401/470 (85%)	388 (97%)	13 (3%)	44	65

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	GLU
1	A	319	SER
1	A	369	LEU
1	A	409	GLU
1	A	451	LEU
1	B	275	GLU
1	B	290	SER
1	B	338	LYS
1	B	347	ASN
1	B	389	GLN
1	B	412	ARG
2	D	695	GLN
2	D	696	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	GLN
1	A	392	GLN
1	A	396	HIS
1	A	437	ASN
1	B	346	ASN
1	B	347	ASN
1	B	389	GLN
1	B	392	GLN
1	B	400	GLN
1	B	437	ASN
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

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	226/251 (90%)	0.05	5 (2%) 62 59	46, 66, 88, 101	0
1	B	225/251 (89%)	0.51	20 (8%) 10 9	47, 76, 101, 102	0
2	C	11/15 (73%)	0.94	2 (18%) 1 1	79, 84, 97, 101	0
2	D	10/15 (66%)	1.12	3 (30%) 1 1	92, 94, 100, 101	0
All	All	472/532 (88%)	0.31	30 (6%) 20 18	46, 71, 100, 102	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	256	THR	5.4
1	B	440	LEU	5.2
1	B	233	PRO	5.2
1	B	252	MET	4.3
1	B	257	VAL	4.1
1	B	451	LEU	4.0
1	A	458	VAL	3.6
1	B	255	PRO	3.5
1	B	251	ALA	3.5
2	C	697	GLY	3.4
2	D	695	GLN	2.9
1	B	250	TYR	2.8
1	B	258	PRO	2.8
1	B	253	PRO	2.8
1	B	254	ASP	2.7
2	D	687	HIS	2.7
1	B	421	LEU	2.7
1	A	442	GLY	2.6
1	B	436	TYR	2.4
1	B	441	GLU	2.4
1	B	330	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	369	LEU	2.4
2	C	695	GLN	2.3
1	B	294	LEU	2.3
1	B	310	ILE	2.2
1	B	442	GLY	2.2
1	B	343	LEU	2.1
1	A	234	TYR	2.1
2	D	696	GLU	2.1
1	A	421	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.