



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:57 AM GMT

PDB ID : 3CTB  
Title : Tethered PXR-LBD/SRC-1p apoprotein  
Authors : Lesburg, C.A.  
Deposited on : 2008-04-11  
Resolution : 2.00 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](mailto: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.

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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 : 1.7 (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

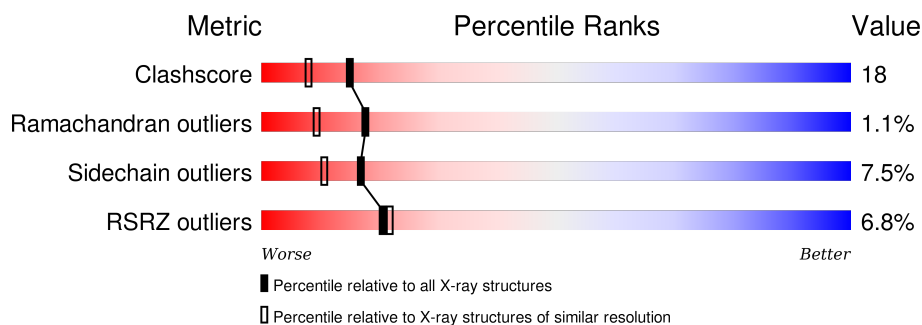
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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  $\geq 3$ , 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	344	<div> <div>4%</div> <div> <div>54%</div> <div>25%</div> <div>• •</div> <div>17%</div> </div> </div>
1	B	344	<div> <div>7%</div> <div> <div>60%</div> <div>19%</div> <div>5%</div> <div>17%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5078 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 Pregnane X receptor, Linker, Steroid receptor coactivator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	2	0
			2369	1520	410	420	19			
1	B	287	Total	C	N	O	S	0	1	0
			2353	1510	406	418	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MET	-	EXPRESSION TAG	UNP O75469
A	120	LYS	-	EXPRESSION TAG	UNP O75469
A	121	LYS	-	EXPRESSION TAG	UNP O75469
A	122	GLY	-	EXPRESSION TAG	UNP O75469
A	123	HIS	-	EXPRESSION TAG	UNP O75469
A	124	HIS	-	EXPRESSION TAG	UNP O75469
A	125	HIS	-	EXPRESSION TAG	UNP O75469
A	126	HIS	-	EXPRESSION TAG	UNP O75469
A	127	HIS	-	EXPRESSION TAG	UNP O75469
A	128	HIS	-	EXPRESSION TAG	UNP O75469
A	129	GLY	-	EXPRESSION TAG	UNP O75469
A	435	GLY	-	LINKER	UNP O75469
A	436	GLY	-	LINKER	UNP O75469
A	437	SER	-	LINKER	UNP O75469
A	438	GLY	-	LINKER	UNP O75469
A	439	GLY	-	LINKER	UNP O75469
B	119	MET	-	EXPRESSION TAG	UNP O75469
B	120	LYS	-	EXPRESSION TAG	UNP O75469
B	121	LYS	-	EXPRESSION TAG	UNP O75469
B	122	GLY	-	EXPRESSION TAG	UNP O75469
B	123	HIS	-	EXPRESSION TAG	UNP O75469
B	124	HIS	-	EXPRESSION TAG	UNP O75469
B	125	HIS	-	EXPRESSION TAG	UNP O75469
B	126	HIS	-	EXPRESSION TAG	UNP O75469
B	127	HIS	-	EXPRESSION TAG	UNP O75469

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Chain	Residue	Modelled	Actual	Comment	Reference
B	128	HIS	-	EXPRESSION TAG	UNP O75469
B	129	GLY	-	EXPRESSION TAG	UNP O75469
B	435	GLY	-	LINKER	UNP O75469
B	436	GLY	-	LINKER	UNP O75469
B	437	SER	-	LINKER	UNP O75469
B	438	GLY	-	LINKER	UNP O75469
B	439	GLY	-	LINKER	UNP O75469

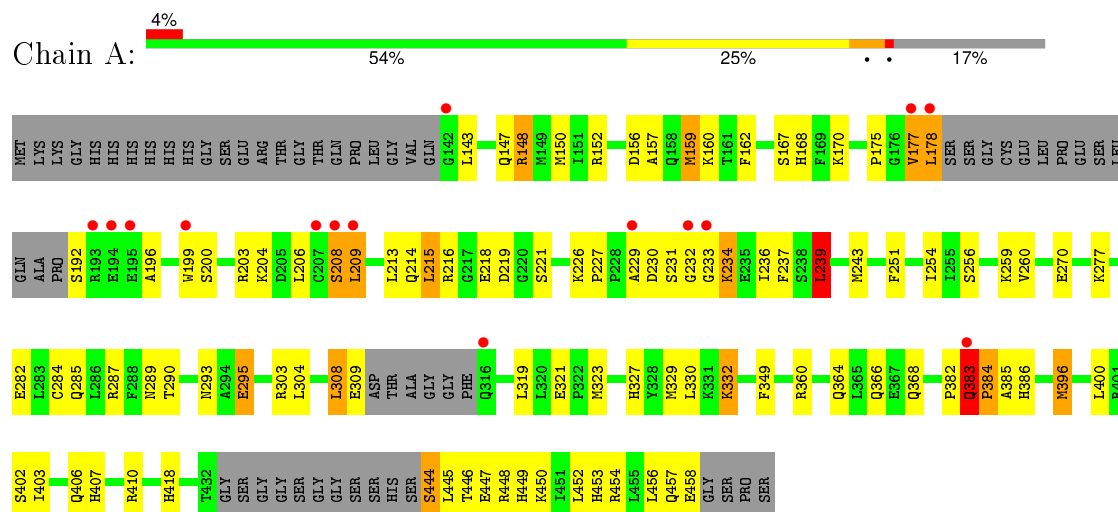
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	184	Total 184	O 184	0	0
2	B	172	Total 172	O 172	0	0

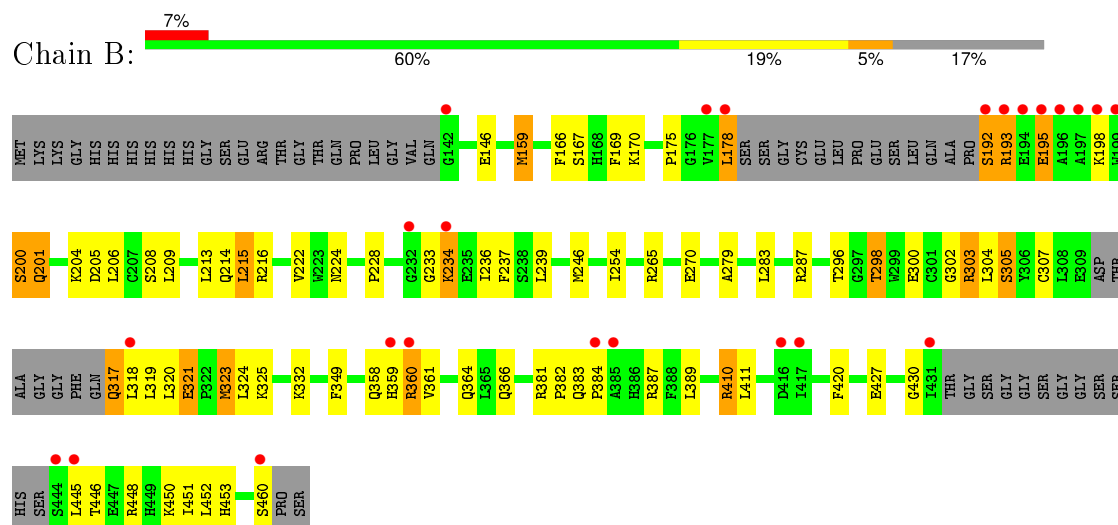
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Pregnane X receptor, Linker, Steroid receptor coactivator 1



- Molecule 1: Pregnane X receptor, Linker, Steroid receptor coactivator 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.24Å 89.24Å 105.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.31 – 2.00 45.32 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.31-2.00) 96.4 (45.32-2.00)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.00Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, $R_{free}$	0.204 , 0.244 0.204 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.5	EDS
Estimated twinning fraction	0.000 for k,h,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 54253 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.66	0/2419	0.70	5/3253 (0.2%)
1	B	0.64	1/2402 (0.0%)	0.70	0/3229
All	All	0.65	1/4821 (0.0%)	0.70	5/6482 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	MET	SD-CE	-7.58	1.35	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	MET	CG-SD-CE	-8.91	85.94	100.20
1	A	383	GLN	C-N-CD	-6.23	106.89	120.60
1	A	396	MET	CG-SD-CE	-5.48	91.42	100.20
1	A	308	LEU	CB-CG-CD1	5.07	119.61	111.00
1	A	239	LEU	CB-CG-CD1	5.01	119.52	111.00

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	2369	0	2387	101	0
1	B	2353	0	2374	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	184	0	0	11	0
2	B	172	0	0	11	0
All	All	5078	0	4761	167	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 (167) 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:170:LYS:HD3	1:B:303:ARG:HH22	1.12	1.09
1:B:317:GLN:HG2	1:B:318:LEU:H	0.93	1.04
1:A:383:GLN:HB2	1:A:384:PRO:HD3	1.38	1.02
1:B:317:GLN:HG2	1:B:318:LEU:N	1.72	0.98
1:A:383:GLN:CB	1:A:384:PRO:HD3	2.01	0.89
1:A:218:GLU:HB2	1:B:178:LEU:HD23	1.58	0.85
1:B:170:LYS:HD3	1:B:303:ARG:NH2	1.94	0.83
1:A:277:LYS:HD2	1:A:449:HIS:CE1	2.14	0.82
1:B:254:ILE:HD11	1:B:287:ARG:HD2	1.60	0.81
1:A:383:GLN:HB2	1:A:384:PRO:CD	2.11	0.81
1:B:317:GLN:CG	1:B:318:LEU:H	1.86	0.79
1:A:382:PRO:HD2	1:A:386:HIS:CD2	2.19	0.78
1:A:215:LEU:HD22	1:A:304:LEU:CD2	2.15	0.76
1:B:200:SER:O	1:B:204:LYS:HG3	1.84	0.76
1:A:206:LEU:HD12	1:A:236:ILE:HD12	1.68	0.76
1:A:383:GLN:O	1:A:385:ALA:N	2.21	0.73
1:B:361:VAL:HG23	2:B:540:HOH:O	1.88	0.73
1:A:383:GLN:CB	1:A:384:PRO:CD	2.66	0.73
1:A:218:GLU:HG2	1:A:303:ARG:NH2	2.05	0.72
1:B:224:ASN:HB2	2:B:628:HOH:O	1.90	0.71
1:B:445:LEU:HD21	2:B:567:HOH:O	1.91	0.70
1:A:218:GLU:HG2	1:A:303:ARG:CZ	2.23	0.69
1:A:233:GLY:O	1:A:236:ILE:HG12	1.93	0.68
1:B:195:GLU:O	1:B:198:LYS:HG2	1.93	0.68
1:A:209:LEU:N	1:A:209:LEU:HD13	2.09	0.67
1:A:157:ALA:HB2	1:A:260:VAL:HG22	1.75	0.67
1:A:216:ARG:HG3	1:A:216:ARG:HH11	1.59	0.67
1:A:329:MET:HB3	1:A:396:MET:HE1	1.77	0.66
1:A:177:VAL:HA	2:A:618:HOH:O	1.94	0.66
1:A:175:PRO:HG3	1:A:239:LEU:HD13	1.76	0.66
1:A:454:ARG:O	1:A:458:GLU:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HD22	1:A:304:LEU:HD21	1.80	0.64
1:B:213:LEU:HD21	1:B:215:LEU:HD12	1.80	0.63
1:B:166:PHE:HD2	1:B:169:PHE:CD2	2.16	0.63
1:A:382:PRO:HD2	1:A:386:HIS:HD2	1.64	0.63
1:A:157:ALA:HB2	1:A:260:VAL:CG2	2.30	0.62
1:A:270:GLU:OE2	1:A:446:THR:HG23	1.99	0.62
1:A:383:GLN:CG	1:A:384:PRO:HD3	2.31	0.61
1:B:296:THR:OG1	1:B:298:THR:HG23	2.00	0.61
1:A:329:MET:HB3	1:A:396:MET:CE	2.31	0.61
1:A:243:MET:HE2	2:A:637:HOH:O	1.99	0.60
1:A:254:ILE:HD11	1:A:287:ARG:HD2	1.83	0.60
1:B:460:SER:HB2	2:B:470:HOH:O	2.02	0.60
1:A:209:LEU:HG	1:A:323:MET:CE	2.31	0.59
1:A:382:PRO:O	1:A:383:GLN:O	2.21	0.59
1:A:157:ALA:CB	1:A:260:VAL:HG22	2.32	0.59
1:B:170:LYS:CD	1:B:303:ARG:HH22	2.01	0.59
1:B:300:GLU:HG2	2:B:627:HOH:O	2.02	0.59
1:B:233:GLY:O	1:B:234:LYS:HB3	2.03	0.59
1:A:445:LEU:O	1:A:449:HIS:HD2	1.87	0.58
1:B:317:GLN:CG	1:B:318:LEU:N	2.57	0.56
1:A:215:LEU:CD2	1:A:304:LEU:HD21	2.35	0.56
1:A:289:ASN:HD22	1:A:327:HIS:HD1	1.51	0.56
1:B:446:THR:HG23	2:B:600:HOH:O	2.04	0.56
1:B:201:GLN:NE2	1:B:205:ASP:OD1	2.39	0.56
1:A:402:SER:O	1:A:406:GLN:HG3	2.07	0.55
1:A:209:LEU:HD21	1:A:410:ARG:NH1	2.21	0.55
1:A:178:LEU:N	1:A:178:LEU:HD23	2.22	0.55
1:B:270:GLU:HB3	1:B:445:LEU:HD12	1.87	0.55
1:A:447:GLU:O	1:A:450:LYS:HE2	2.07	0.55
1:A:175:PRO:CG	1:A:239:LEU:HD13	2.36	0.55
1:B:214:GLN:HE21	1:B:216:ARG:HH11	1.54	0.55
1:A:444:SER:O	1:A:448:ARG:HG3	2.06	0.55
1:A:216:ARG:HG3	1:A:216:ARG:NH1	2.23	0.54
1:A:332:LYS:HG2	2:A:616:HOH:O	2.07	0.54
1:A:368:GLN:HG3	2:A:603:HOH:O	2.07	0.54
1:A:214:GLN:HE21	1:A:216:ARG:HH11	1.54	0.54
1:A:208:SER:C	1:A:209:LEU:HD13	2.27	0.54
1:A:206:LEU:CD1	1:A:236:ILE:HD12	2.38	0.53
1:A:206:LEU:HD11	1:A:237:PHE:CE2	2.44	0.53
1:B:234:LYS:HA	1:B:237:PHE:HD1	1.74	0.53
1:A:168:HIS:HD2	2:A:638:HOH:O	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ASP:OD2	1:A:160:LYS:HE2	2.09	0.53
1:A:148:ARG:HD3	2:A:640:HOH:O	2.08	0.52
1:A:209:LEU:HD11	1:A:321:GLU:HG2	1.91	0.52
1:A:157:ALA:HA	1:A:260:VAL:HG21	1.91	0.52
1:A:209:LEU:CD1	1:A:321:GLU:HG2	2.40	0.52
1:A:200:SER:O	1:A:204:LYS:HG3	2.09	0.51
1:B:215:LEU:HD12	1:B:304:LEU:HD23	1.92	0.51
1:A:177:VAL:HG12	1:B:215:LEU:CD2	2.41	0.51
1:A:156:ASP:CG	1:A:160:LYS:HE2	2.30	0.51
1:B:360:ARG:O	1:B:364:GLN:HG2	2.11	0.51
1:A:293:ASN:OD1	1:A:295:GLU:HG2	2.11	0.51
1:B:411:LEU:CD1	1:B:420:PHE:CZ	2.93	0.51
1:A:219:ASP:H	1:B:178:LEU:HD22	1.76	0.50
1:A:156:ASP:OD1	1:A:160:LYS:HE2	2.12	0.50
1:A:234:LYS:HE2	1:A:237:PHE:HE1	1.76	0.50
1:B:213:LEU:HD21	1:B:215:LEU:CD1	2.41	0.50
1:B:166:PHE:HD2	1:B:169:PHE:HD2	1.60	0.49
1:A:177:VAL:HG12	1:B:215:LEU:HD21	1.94	0.49
1:A:157:ALA:CB	1:A:260:VAL:CG2	2.90	0.49
1:B:166:PHE:HE2	1:B:246:MET:HG2	1.76	0.49
1:B:234:LYS:HA	1:B:237:PHE:CD1	2.47	0.49
1:A:229:ALA:HB1	2:A:621:HOH:O	2.12	0.49
1:B:175:PRO:HG3	1:B:239:LEU:HD23	1.94	0.48
1:B:167:SER:O	1:B:170:LYS:HE2	2.13	0.48
1:A:251:PHE:CD2	1:A:284[A]:CYS:SG	3.07	0.48
1:B:382:PRO:HG2	1:B:383:GLN:NE2	2.28	0.48
1:B:206:LEU:HD12	1:B:236:ILE:HD12	1.95	0.48
1:B:383:GLN:CD	1:B:383:GLN:H	2.16	0.48
1:B:319:LEU:HD22	1:B:325:LYS:HA	1.95	0.48
1:A:403:ILE:O	1:A:407[B]:HIS:HD2	1.97	0.48
1:A:418:HIS:HE1	2:A:568:HOH:O	1.96	0.47
1:A:234:LYS:NZ	1:A:418:HIS:HD2	2.13	0.47
1:A:150:MET:CE	1:A:368:GLN:NE2	2.77	0.47
1:B:430:GLY:HA2	2:B:613:HOH:O	2.15	0.47
1:B:192:SER:O	1:B:193:ARG:O	2.33	0.47
1:A:148:ARG:HB2	1:A:148:ARG:HE	1.59	0.46
1:A:221:SER:HB3	1:B:228:PRO:HD3	1.97	0.46
1:A:150:MET:HE1	1:A:368:GLN:NE2	2.30	0.46
1:B:216:ARG:HG2	1:B:222:VAL:HG22	1.97	0.46
1:A:290:THR:HG21	2:A:495:HOH:O	2.14	0.46
1:A:218:GLU:CG	1:A:303:ARG:NH1	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:HIS:O	1:A:457:GLN:HB2	2.16	0.46
1:B:254:ILE:CD1	1:B:287:ARG:HD2	2.38	0.46
1:B:214:GLN:HB3	1:B:305:SER:HB2	1.98	0.45
1:A:209:LEU:HD22	1:A:209:LEU:H	1.80	0.45
1:B:209:LEU:HD21	1:B:321:GLU:HG3	1.98	0.45
1:A:178:LEU:CD2	1:A:178:LEU:N	2.80	0.45
1:B:453:HIS:HD2	2:B:543:HOH:O	1.99	0.45
1:A:323:MET:CE	1:A:407[B]:HIS:CE1	3.00	0.45
1:B:427:GLU:OE2	1:B:451:ILE:HG13	2.16	0.45
1:A:349:PHE:O	1:A:366:GLN:HB2	2.18	0.44
1:A:332:LYS:HD2	2:A:607:HOH:O	2.17	0.44
1:B:358:GLN:HB3	1:B:361:VAL:CG2	2.48	0.44
1:A:177:VAL:CG1	1:B:215:LEU:HD21	2.46	0.44
1:A:282:GLU:HG2	1:A:400:LEU:HG	1.99	0.44
1:B:359:HIS:HB2	2:B:591:HOH:O	2.17	0.44
1:B:169:PHE:O	1:B:303:ARG:NH2	2.48	0.44
1:A:259:LYS:HD2	1:A:456:LEU:HA	1.98	0.44
1:B:453:HIS:HE1	2:B:565:HOH:O	2.00	0.44
1:A:143:LEU:HD22	1:A:147:GLN:HB3	2.00	0.44
1:A:227:PRO:HG2	1:A:309:GLU:OE1	2.18	0.44
1:A:230:ASP:N	2:A:621:HOH:O	2.34	0.43
1:B:452:LEU:HA	1:B:452:LEU:HD23	1.83	0.43
1:A:285:GLN:NE2	1:A:327:HIS:NE2	2.66	0.43
1:B:411:LEU:CD1	1:B:420:PHE:HZ	2.31	0.43
1:A:192:SER:O	1:A:196:ALA:HB2	2.19	0.43
1:A:231:SER:HB3	1:A:232:GLY:H	1.57	0.43
1:A:199:TRP:O	1:A:203:ARG:HG3	2.17	0.43
1:B:384:PRO:HA	1:B:387:ARG:HG3	2.01	0.43
1:B:321:GLU:OE1	1:B:410:ARG:NH2	2.39	0.42
1:A:167:SER:O	1:A:170:LYS:HE3	2.18	0.42
1:B:166:PHE:CD2	1:B:169:PHE:CD2	3.03	0.42
1:B:215:LEU:HD12	1:B:304:LEU:CD2	2.48	0.42
1:B:296:THR:O	1:B:298:THR:HG22	2.20	0.42
1:B:201:GLN:HE21	1:B:205:ASP:CG	2.23	0.42
1:A:256:SER:O	1:A:260:VAL:HG13	2.18	0.42
1:B:298:THR:HB	1:B:307:CYS:HA	2.01	0.42
1:A:383:GLN:CG	1:A:384:PRO:CD	2.96	0.42
1:B:146:GLU:HB2	2:B:598:HOH:O	2.20	0.41
1:A:277:LYS:HB3	1:A:277:LYS:HE3	1.52	0.41
1:B:193:ARG:C	1:B:195:GLU:H	2.22	0.41
1:B:216:ARG:HH11	1:B:216:ARG:HG3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:HE2	1:A:237:PHE:CE1	2.55	0.41
1:B:381:ARG:HD3	1:B:389:LEU:HD23	2.02	0.41
1:B:349:PHE:O	1:B:366:GLN:HB2	2.20	0.41
1:A:360:ARG:O	1:A:364:GLN:HG3	2.21	0.41
1:B:206:LEU:HD11	1:B:237:PHE:CE2	2.55	0.41
1:A:213:LEU:C	1:A:213:LEU:HD23	2.42	0.41
1:A:209:LEU:HG	1:A:323:MET:HE3	2.02	0.40
1:B:323:MET:HA	1:B:323:MET:HE3	2.02	0.40
1:A:214:GLN:HE21	1:A:216:ARG:NH1	2.17	0.40
1:A:208:SER:HB2	1:A:209:LEU:HD13	2.04	0.40
1:A:330:LEU:N	1:A:396:MET:HE3	2.37	0.40
1:B:279:ALA:HB1	1:B:283:LEU:HD13	2.04	0.40
1:A:215:LEU:HD22	1:A:304:LEU:HD23	1.95	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	281/344 (82%)	272 (97%)	6 (2%)	3 (1%)	17	9
1	B	280/344 (81%)	267 (95%)	10 (4%)	3 (1%)	17	9
All	All	561/688 (82%)	539 (96%)	16 (3%)	6 (1%)	17	9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	GLN
1	A	384	PRO
1	B	193	ARG
1	A	234	LYS
1	B	302	GLY

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Mol	Chain	Res	Type
1	B	234	LYS

### 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	262/302 (87%)	245 (94%)	17 (6%)	21	15
1	B	260/302 (86%)	238 (92%)	22 (8%)	13	8
All	All	522/604 (86%)	483 (92%)	39 (8%)	17	11

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	152	ARG
1	A	159	MET
1	A	162	PHE
1	A	177	VAL
1	A	178	LEU
1	A	208	SER
1	A	209	LEU
1	A	215	LEU
1	A	226	LYS
1	A	239	LEU
1	A	295	GLU
1	A	308	LEU
1	A	319	LEU
1	A	332	LYS
1	A	444	SER
1	A	452	LEU
1	B	159	MET
1	B	178	LEU
1	B	192	SER
1	B	195	GLU
1	B	200	SER

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Mol	Chain	Res	Type
1	B	201	GLN
1	B	208	SER
1	B	215	LEU
1	B	265	ARG
1	B	298	THR
1	B	303	ARG
1	B	305	SER
1	B	317	GLN
1	B	320	LEU
1	B	321	GLU
1	B	323	MET
1	B	324	LEU
1	B	332	LYS
1	B	360	ARG
1	B	410	ARG
1	B	448	ARG
1	B	450	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	214	GLN
1	A	272	GLN
1	A	285	GLN
1	A	368	GLN
1	A	386	HIS
1	A	418	HIS
1	A	449	HIS
1	A	453	HIS
1	B	201	GLN
1	B	214	GLN
1	B	224	ASN
1	B	272	GLN
1	B	383	GLN
1	B	386	HIS
1	B	453	HIS
1	B	457	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, 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	287/344 (83%)	0.27	15 (5%) 31 33	29, 46, 81, 123	0
1	B	287/344 (83%)	0.40	24 (8%) 14 14	30, 47, 87, 143	0
All	All	574/688 (83%)	0.34	39 (6%) 20 22	29, 47, 85, 143	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	LEU	7.4
1	B	193	ARG	5.7
1	B	192	SER	5.3
1	B	194	GLU	5.1
1	A	177	VAL	4.6
1	A	232	GLY	4.5
1	B	196	ALA	4.4
1	A	194	GLU	4.3
1	A	207	CYS	4.1
1	B	444	SER	3.9
1	A	208	SER	3.8
1	B	198	LYS	3.8
1	B	417	ILE	3.7
1	B	195	GLU	3.5
1	A	193	ARG	3.4
1	B	384	PRO	3.3
1	B	197	ALA	3.3
1	A	178	LEU	3.0
1	A	383	GLN	2.9
1	B	178	LEU	2.9
1	B	360	ARG	2.8
1	B	385	ALA	2.7
1	B	234	LYS	2.7
1	B	460	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	142	GLY	2.7
1	B	199	TRP	2.6
1	B	359	HIS	2.6
1	A	316	GLN	2.5
1	B	232	GLY	2.3
1	B	142	GLY	2.2
1	B	431	ILE	2.2
1	A	229	ALA	2.2
1	B	445	LEU	2.2
1	A	199	TRP	2.2
1	B	177	VAL	2.1
1	B	318	LEU	2.1
1	A	233	GLY	2.0
1	B	416	ASP	2.0
1	A	195	GLU	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.