



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:08 AM GMT

PDB ID : 2FSZ
Title : A second binding site for hydroxytamoxifen within the coactivator-binding groove of estrogen receptor beta
Authors : Wang, Yong
Deposited on : 2006-01-23
Resolution : 2.20 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
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

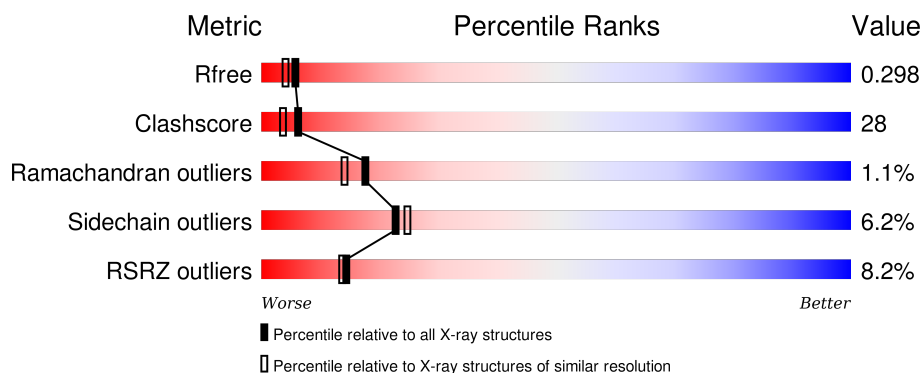
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	246	<div> <div>8%</div> <div>49%</div> <div>38%</div> <div>•</div> <div>9%</div> </div>
1	B	246	<div> <div>7%</div> <div>54%</div> <div>35%</div> <div>•</div> <div>8%</div> </div>

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
2	OHT	A	101	-	-	-	X
2	OHT	B	102	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3717 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.

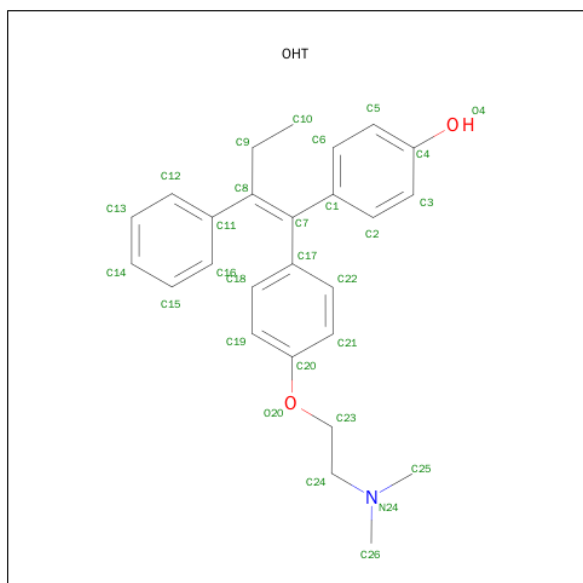
- Molecule 1 is a protein called Estrogen receptor beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1766	1136	300	313	17			
1	B	227	Total	C	N	O	S	0	0	0
			1795	1155	304	319	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	SER	CYS	ENGINEERED	UNP Q92731
A	369	SER	CYS	ENGINEERED	UNP Q92731
A	481	SER	CYS	ENGINEERED	UNP Q92731
B	334	SER	CYS	ENGINEERED	UNP Q92731
B	369	SER	CYS	ENGINEERED	UNP Q92731
B	481	SER	CYS	ENGINEERED	UNP Q92731

- Molecule 2 is 4-HYDROXYTAMOXIFEN (three-letter code: OHT) (formula: C₂₆H₂₉NO₂).



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

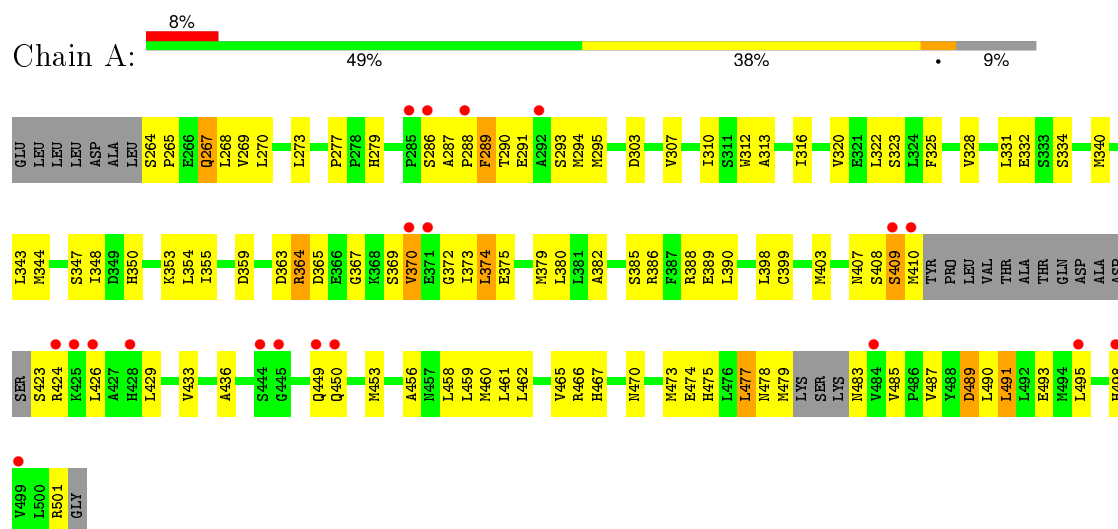
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	23	Total	O	0	0
			23	23		

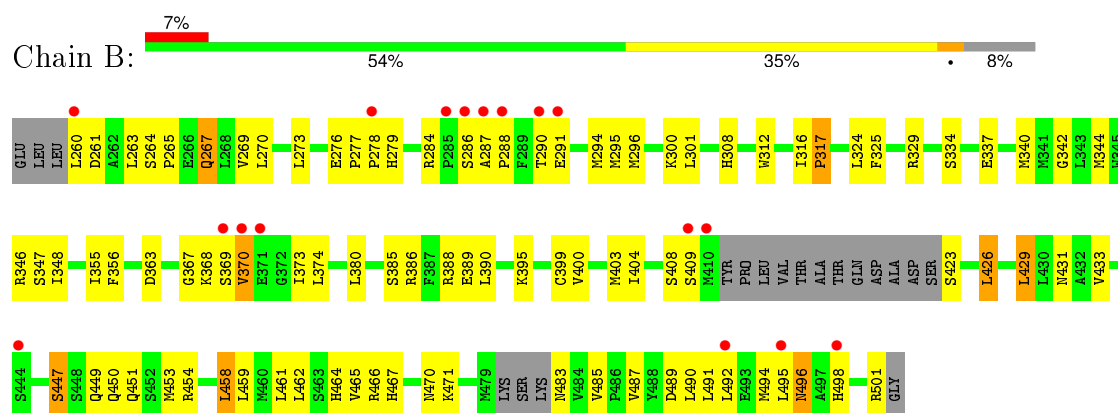
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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 beta



• Molecule 1: Estrogen receptor beta



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	105.04Å 105.04Å 102.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.11 – 2.20 19.16 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.11-2.20) 96.8 (19.16-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.45 (at 2.21Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.273 , 0.299 0.271 , 0.298	Depositor DCC
R_{free} test set	1019 reflections (3.88%)	DCC
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.7	EDS
Estimated twinning fraction	0.068 for l,-k,h 0.067 for -l,-k,-h 0.065 for -h,-l,-k 0.065 for -h,l,k 0.365 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 27272 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3717	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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](#)

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

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	0.38	0/1797	0.61	1/2425 (0.0%)
1	B	0.37	0/1826	0.61	0/2465
All	All	0.37	0/3623	0.61	1/4890 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	ARG	NE-CZ-NH2	-6.01	117.30	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	1766	0	1843	111	0
1	B	1795	0	1874	112	0
2	A	58	0	57	1	0
2	B	58	0	57	3	0
3	A	17	0	0	1	0
3	B	23	0	0	5	0
All	All	3717	0	3831	210	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 28.

All (210) 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:A:270:LEU:HA	1:A:273:LEU:HD12	1.36	1.06
1:B:370:VAL:HG23	1:B:373:ILE:HG12	1.32	1.05
1:A:347:SER:HA	1:A:355:ILE:HD13	1.44	0.99
1:A:423:SER:HB2	1:A:426:LEU:HD13	1.44	0.96
1:B:291:GLU:HG3	1:B:370:VAL:HA	1.47	0.94
1:A:386:ARG:HG3	1:A:461:LEU:HD11	1.51	0.92
1:B:426:LEU:H	1:B:426:LEU:HD12	1.37	0.90
1:A:399:CYS:O	1:A:403:MET:HG3	1.75	0.86
1:A:410:MET:SD	1:B:386:ARG:HG3	2.20	0.80
1:B:290:THR:HG22	1:B:291:GLU:H	1.46	0.80
1:B:423:SER:HB2	1:B:426:LEU:HD13	1.63	0.79
1:A:370:VAL:HG23	1:A:373:ILE:HG12	1.62	0.79
1:B:261:ASP:O	1:B:267:GLN:HG3	1.83	0.78
1:B:370:VAL:HG23	1:B:373:ILE:CG1	2.14	0.76
1:A:386:ARG:CG	1:A:461:LEU:HD11	2.15	0.76
1:B:290:THR:HG22	1:B:291:GLU:N	2.01	0.75
1:B:347:SER:HA	1:B:355:ILE:HD13	1.67	0.75
1:B:334:SER:HB3	1:B:408:SER:OG	1.87	0.75
1:A:334:SER:HB3	1:A:408:SER:HB3	1.68	0.74
1:B:487:VAL:HG12	1:B:491:LEU:HD13	1.70	0.74
1:B:395:LYS:HG3	3:B:8:HOH:O	1.89	0.72
1:A:355:ILE:N	1:A:355:ILE:HD12	2.04	0.72
1:A:466:ARG:HH11	1:B:467:HIS:HB2	1.55	0.71
1:B:355:ILE:HD12	1:B:355:ILE:N	2.05	0.71
1:A:370:VAL:HG23	1:A:373:ILE:CG1	2.22	0.70
1:A:295:MET:HE1	2:A:101:OHT:H13	1.73	0.70
1:B:287:ALA:HB1	1:B:288:PRO:HD2	1.72	0.70
1:B:426:LEU:H	1:B:426:LEU:CD1	2.04	0.70
1:B:368:LYS:HG2	1:B:374:LEU:HD11	1.74	0.70
1:A:375:GLU:O	1:A:379:MET:HG3	1.92	0.69
1:A:373:ILE:C	1:A:373:ILE:HD12	2.12	0.69
1:B:370:VAL:CG2	1:B:373:ILE:HG12	2.17	0.69
1:B:270:LEU:HA	1:B:273:LEU:HD12	1.75	0.69
1:A:287:ALA:HB1	1:A:288:PRO:HD2	1.74	0.69
1:B:373:ILE:HD12	1:B:373:ILE:C	2.13	0.68
1:B:260:LEU:HG	1:B:261:ASP:N	2.09	0.68
1:B:301:LEU:HD21	1:B:356:PHE:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ASN:HD22	1:B:470:ASN:ND2	1.91	0.67
1:A:350:HIS:HB2	1:A:355:ILE:HD11	1.76	0.67
1:A:268:LEU:HD23	1:A:436:ALA:HB2	1.75	0.67
1:B:367:GLY:HA3	1:B:373:ILE:HD11	1.76	0.66
1:A:347:SER:CA	1:A:355:ILE:HD13	2.25	0.66
1:A:456:ALA:O	1:A:460:MET:HG3	1.95	0.66
1:A:334:SER:HB3	1:A:408:SER:CB	2.25	0.66
1:A:426:LEU:HD12	1:A:426:LEU:H	1.62	0.65
1:A:310:ILE:HD13	1:A:331:LEU:HD13	1.79	0.65
1:B:400:VAL:O	1:B:404:ILE:HG13	1.96	0.65
1:A:386:ARG:HG2	1:A:461:LEU:HD21	1.80	0.64
1:B:367:GLY:CA	1:B:373:ILE:HD11	2.27	0.64
1:A:487:VAL:HG12	1:A:491:LEU:HD13	1.79	0.64
1:A:325:PHE:HB2	1:A:501:ARG:HD2	1.81	0.63
1:A:373:ILE:HD12	1:A:374:LEU:N	2.12	0.63
1:A:370:VAL:CG2	1:A:373:ILE:HG12	2.28	0.62
1:A:470:ASN:HD22	1:B:470:ASN:HD22	1.47	0.62
1:A:423:SER:N	1:A:426:LEU:HD22	2.14	0.62
1:A:340:MET:O	1:A:344:MET:HG3	2.00	0.62
1:B:373:ILE:HD12	1:B:374:LEU:N	2.15	0.61
1:B:296:MET:CE	1:B:300:LYS:HD2	2.30	0.61
1:B:290:THR:CG2	1:B:291:GLU:H	2.13	0.61
1:A:367:GLY:CA	1:A:373:ILE:HD11	2.30	0.61
1:A:372:GLY:HA3	1:A:475:HIS:HE2	1.63	0.61
1:B:265:PRO:O	1:B:269:VAL:HG23	2.00	0.61
1:B:454:ARG:HG2	1:B:458:LEU:HD22	1.84	0.60
1:B:466:ARG:HH11	1:B:466:ARG:HG2	1.66	0.60
1:A:268:LEU:HD21	1:A:433:VAL:HA	1.83	0.59
1:B:294:MET:CE	1:B:369:SER:HB2	2.32	0.59
1:A:426:LEU:H	1:A:426:LEU:CD1	2.16	0.59
1:B:449:GLN:O	1:B:453:MET:HG3	2.03	0.59
1:B:426:LEU:N	1:B:426:LEU:HD12	2.13	0.58
1:B:296:MET:HE1	1:B:300:LYS:HD2	1.86	0.58
1:A:367:GLY:HA3	1:A:373:ILE:HD11	1.84	0.58
1:A:409:SER:O	1:A:410:MET:HG3	2.04	0.58
1:A:364:ARG:HH12	1:B:492:LEU:HD22	1.68	0.58
1:B:278:PRO:HG2	1:B:308:HIS:CE1	2.38	0.58
1:A:483:ASN:HA	3:A:13:HOH:O	2.04	0.58
1:B:334:SER:HB3	1:B:408:SER:CB	2.33	0.57
1:B:390:LEU:HB3	3:B:45:HOH:O	2.04	0.57
1:B:485:VAL:O	1:B:487:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:PHE:HB2	1:B:501:ARG:HD2	1.86	0.56
1:A:320:VAL:HG12	1:A:320:VAL:O	2.05	0.56
1:A:390:LEU:HD13	1:A:458:LEU:HD12	1.88	0.56
1:B:267:GLN:HE21	1:B:267:GLN:HA	1.70	0.55
1:A:364:ARG:NH1	1:B:492:LEU:HD22	2.21	0.55
1:B:367:GLY:C	1:B:373:ILE:HD11	2.28	0.54
1:B:294:MET:HE3	1:B:369:SER:HB2	1.90	0.54
1:B:380:LEU:HD11	2:B:102:OHT:H101	1.89	0.54
1:B:368:LYS:HG2	1:B:374:LEU:CD1	2.37	0.54
1:A:410:MET:CE	1:B:386:ARG:HD2	2.38	0.54
1:B:324:LEU:HD11	2:B:104:OHT:H263	1.90	0.54
1:A:290:THR:HG22	1:A:291:GLU:N	2.24	0.53
1:A:450:GLN:HA	1:A:453:MET:HE2	1.90	0.53
1:B:294:MET:HG2	1:B:370:VAL:HG22	1.89	0.53
1:A:268:LEU:HD23	1:A:436:ALA:CB	2.39	0.53
1:A:410:MET:SD	1:B:386:ARG:HD2	2.48	0.53
1:B:301:LEU:CD2	1:B:356:PHE:HB3	2.39	0.53
1:B:487:VAL:O	1:B:487:VAL:HG12	2.09	0.52
1:B:423:SER:CB	1:B:426:LEU:HD13	2.38	0.52
1:B:325:PHE:HB2	1:B:501:ARG:HB2	1.90	0.52
1:B:385:SER:O	1:B:389:GLU:HG2	2.09	0.52
1:A:426:LEU:HD12	1:A:426:LEU:N	2.23	0.52
1:B:466:ARG:NH1	1:B:466:ARG:HG2	2.25	0.52
1:A:475:HIS:HA	1:A:478:ASN:HD22	1.75	0.52
1:A:350:HIS:CB	1:A:355:ILE:HD11	2.40	0.51
1:A:328:VAL:O	1:A:332:GLU:HB2	2.11	0.51
1:B:355:ILE:N	1:B:355:ILE:CD1	2.74	0.51
1:A:289:PHE:CE1	1:A:294:MET:HA	2.45	0.51
1:A:501:ARG:HG3	1:A:501:ARG:HH11	1.76	0.51
1:B:348:ILE:O	1:B:388:ARG:HD3	2.10	0.51
1:A:355:ILE:N	1:A:355:ILE:CD1	2.72	0.50
1:A:487:VAL:HG13	1:A:490:LEU:HD23	1.93	0.50
1:A:385:SER:O	1:A:389:GLU:OE1	2.30	0.50
1:B:342:GLY:O	1:B:346:ARG:HG2	2.12	0.49
1:A:423:SER:HB2	1:A:426:LEU:CD1	2.30	0.49
1:A:449:GLN:OE1	1:A:453:MET:HG3	2.12	0.49
1:B:490:LEU:O	1:B:494:MET:HG3	2.13	0.49
1:B:312:TRP:CZ2	1:B:316:ILE:HD11	2.47	0.49
1:A:410:MET:SD	1:B:386:ARG:CG	2.97	0.49
1:A:273:LEU:HD23	1:A:398:LEU:HD11	1.94	0.49
1:A:373:ILE:CD1	1:A:373:ILE:C	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:HG3	1:B:329:ARG:HH11	1.78	0.49
1:A:310:ILE:CD1	1:A:331:LEU:HD13	2.43	0.48
1:A:264:SER:HB2	1:A:267:GLN:HG2	1.94	0.48
1:A:343:LEU:HD23	1:A:380:LEU:HD13	1.95	0.48
1:B:368:LYS:CG	1:B:374:LEU:HD11	2.42	0.48
1:B:260:LEU:CG	1:B:261:ASP:N	2.76	0.48
1:A:470:ASN:ND2	1:B:470:ASN:HD22	2.09	0.48
1:B:447:SER:O	1:B:451:GLN:HG3	2.14	0.48
1:B:264:SER:HB2	1:B:267:GLN:CG	2.44	0.48
1:A:325:PHE:HB2	1:A:501:ARG:CD	2.44	0.48
1:A:277:PRO:HG3	1:A:312:TRP:HB2	1.94	0.48
1:B:390:LEU:HD22	3:B:45:HOH:O	2.13	0.48
1:B:329:ARG:NH1	1:B:329:ARG:HG3	2.29	0.47
1:B:294:MET:HE2	1:B:369:SER:HB2	1.97	0.47
1:A:265:PRO:O	1:A:269:VAL:HG23	2.13	0.47
1:A:495:LEU:HD23	1:A:495:LEU:O	2.14	0.47
1:B:290:THR:CG2	1:B:291:GLU:N	2.69	0.47
1:B:269:VAL:O	1:B:273:LEU:HG	2.14	0.47
1:B:284:ARG:NH1	3:B:44:HOH:O	2.47	0.47
1:A:367:GLY:C	1:A:373:ILE:HD11	2.35	0.47
1:A:466:ARG:HG2	1:A:466:ARG:HH11	1.78	0.47
1:A:295:MET:HG2	1:A:479:MET:SD	2.55	0.47
1:A:303:ASP:O	1:A:307:VAL:HG23	2.13	0.47
1:B:337:GLU:CD	1:B:466:ARG:HE	2.18	0.46
1:A:487:VAL:HG12	1:A:487:VAL:O	2.16	0.46
1:A:467:HIS:HB2	1:B:466:ARG:HH11	1.80	0.46
1:B:459:LEU:O	1:B:462:LEU:HG	2.16	0.46
1:B:294:MET:HG2	1:B:370:VAL:CG2	2.45	0.46
1:A:367:GLY:O	1:A:373:ILE:HD11	2.16	0.46
1:A:291:GLU:HG3	1:A:370:VAL:HG12	1.96	0.46
1:A:267:GLN:HE21	1:A:267:GLN:HA	1.80	0.46
1:B:284:ARG:H	1:B:284:ARG:HG3	1.50	0.46
1:A:475:HIS:CE1	1:A:479:MET:HE2	2.50	0.45
1:B:334:SER:HB3	1:B:408:SER:HB2	1.97	0.45
1:B:340:MET:O	1:B:344:MET:HG3	2.16	0.45
1:A:264:SER:HB2	1:A:267:GLN:CG	2.47	0.45
1:B:483:ASN:N	1:B:483:ASN:ND2	2.64	0.45
1:A:382:ALA:O	1:A:385:SER:HB3	2.17	0.45
1:B:295:MET:HE1	1:B:370:VAL:HG11	1.98	0.45
1:A:353:LYS:HE2	1:A:363:ASP:OD1	2.17	0.45
1:A:313:ALA:HA	1:A:316:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:MET:HE1	1:A:467:HIS:CD2	2.52	0.45
1:B:367:GLY:C	1:B:369:SER:H	2.21	0.44
1:B:423:SER:HB2	1:B:426:LEU:CD1	2.42	0.44
1:A:291:GLU:HG3	1:A:370:VAL:HA	1.98	0.44
1:A:407:ASN:ND2	1:B:464:HIS:HE1	2.16	0.44
1:A:458:LEU:O	1:A:461:LEU:HB2	2.18	0.44
1:B:429:LEU:O	1:B:433:VAL:HG23	2.18	0.44
1:B:501:ARG:HH11	1:B:501:ARG:HG3	1.81	0.44
1:B:450:GLN:HG2	1:B:453:MET:CE	2.48	0.44
1:A:485:VAL:O	1:A:487:VAL:HG23	2.18	0.44
1:A:348:ILE:O	1:A:388:ARG:HD3	2.18	0.44
1:B:461:LEU:O	1:B:465:VAL:HG23	2.18	0.44
1:B:264:SER:HB2	1:B:267:GLN:HG2	2.00	0.43
1:B:373:ILE:CD1	1:B:373:ILE:C	2.83	0.43
1:B:276:GLU:HA	1:B:277:PRO:HD3	1.91	0.43
1:B:261:ASP:C	1:B:263:LEU:N	2.71	0.43
1:B:431:ASN:HB3	3:B:49:HOH:O	2.18	0.43
1:A:473:MET:O	1:A:477:LEU:HB2	2.19	0.43
1:A:322:LEU:O	1:A:323:SER:C	2.55	0.43
1:A:290:THR:H	1:A:293:SER:HG	1.65	0.42
1:B:483:ASN:HD22	1:B:483:ASN:N	2.15	0.42
1:A:403:MET:HE3	1:A:403:MET:HB3	1.85	0.42
1:B:461:LEU:HA	1:B:461:LEU:HD23	1.87	0.42
1:A:489:ASP:N	1:A:489:ASP:OD1	2.51	0.42
1:A:461:LEU:O	1:A:465:VAL:HG23	2.20	0.42
1:B:347:SER:CA	1:B:355:ILE:HD13	2.42	0.42
1:B:495:LEU:O	1:B:495:LEU:HD23	2.20	0.42
1:A:474:GLU:O	1:A:478:ASN:ND2	2.53	0.41
1:A:493:GLU:HA	1:A:493:GLU:OE2	2.19	0.41
1:A:325:PHE:CB	1:A:501:ARG:HD2	2.49	0.41
1:B:380:LEU:CD1	2:B:102:OHT:H101	2.50	0.41
1:A:320:VAL:CG1	1:A:320:VAL:O	2.69	0.41
1:B:471:LYS:HD3	1:B:471:LYS:HA	1.82	0.41
1:A:268:LEU:CD2	1:A:433:VAL:HA	2.51	0.41
1:A:487:VAL:CG1	1:A:491:LEU:HD13	2.49	0.41
1:A:466:ARG:HG2	1:A:466:ARG:NH1	2.35	0.41
1:B:459:LEU:HD22	1:B:462:LEU:HD11	2.02	0.41
1:A:410:MET:SD	1:B:386:ARG:CD	3.09	0.41
1:A:291:GLU:HA	1:A:369:SER:O	2.20	0.41
1:B:340:MET:HG2	1:B:380:LEU:HD21	2.02	0.41
1:B:291:GLU:HG3	1:B:370:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:GLN:HG2	1:A:453:MET:CE	2.50	0.41
1:B:492:LEU:O	1:B:496:ASN:HB2	2.21	0.41
1:B:423:SER:N	1:B:426:LEU:HD22	2.36	0.40
1:A:475:HIS:CE1	1:A:479:MET:CE	3.04	0.40
1:A:462:LEU:HD23	1:A:462:LEU:HA	1.79	0.40
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.93	0.40
1:A:403:MET:HE1	1:A:459:LEU:HD21	2.03	0.40
1:A:370:VAL:HG23	1:A:373:ILE:HG13	2.02	0.40
1:B:399:CYS:O	1:B:403:MET:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/246 (88%)	198 (91%)	17 (8%)	2 (1%)	21	19
1	B	221/246 (90%)	201 (91%)	17 (8%)	3 (1%)	14	10
All	All	438/492 (89%)	399 (91%)	34 (8%)	5 (1%)	17	14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	447	SER
1	A	286	SER
1	B	286	SER
1	B	317	PRO
1	A	424	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	201/220 (91%)	188 (94%)	13 (6%)	21	23
1	B	204/220 (93%)	192 (94%)	12 (6%)	24	27
All	All	405/440 (92%)	380 (94%)	25 (6%)	23	25

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	A	279	HIS
1	A	289	PHE
1	A	359	ASP
1	A	365	ASP
1	A	370	VAL
1	A	374	LEU
1	A	409	SER
1	A	429	LEU
1	A	477	LEU
1	A	489	ASP
1	A	491	LEU
1	A	498	HIS
1	B	267	GLN
1	B	279	HIS
1	B	317	PRO
1	B	363	ASP
1	B	370	VAL
1	B	409	SER
1	B	426	LEU
1	B	429	LEU
1	B	458	LEU
1	B	489	ASP
1	B	496	ASN
1	B	498	HIS

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	267	GLN
1	A	407	ASN
1	A	457	ASN
1	A	464	HIS
1	A	470	ASN
1	A	478	ASN
1	A	483	ASN
1	B	267	GLN
1	B	457	ASN
1	B	464	HIS
1	B	483	ASN

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](#)

4 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	$\# Z > 2$
2	OHT	A	101	-	31,31,31	3.41	21 (67%)	41,41,41	1.59	7 (17%)
2	OHT	A	103	-	31,31,31	3.51	23 (74%)	41,41,41	1.42	6 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OHT	B	102	-	31,31,31	3.43	22 (70%)	41,41,41	1.53	8 (19%)
2	OHT	B	104	-	31,31,31	3.48	21 (67%)	41,41,41	1.50	8 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OHT	A	101	-	-	0/24/24/24	0/3/3/3
2	OHT	A	103	-	-	0/24/24/24	0/3/3/3
2	OHT	B	102	-	-	0/24/24/24	0/3/3/3
2	OHT	B	104	-	-	0/24/24/24	0/3/3/3

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	103	OHT	O20-C20	2.04	1.42	1.37
2	B	102	OHT	C3-C4	2.04	1.43	1.38
2	A	103	OHT	C9-C8	2.07	1.57	1.52
2	B	102	OHT	C21-C20	2.22	1.43	1.38
2	B	102	OHT	C9-C8	2.22	1.57	1.52
2	A	101	OHT	C3-C4	2.26	1.43	1.38
2	B	104	OHT	C21-C20	2.31	1.43	1.38
2	A	103	OHT	C21-C20	2.38	1.43	1.38
2	A	103	OHT	C13-C14	2.57	1.44	1.38
2	B	104	OHT	C3-C4	2.61	1.44	1.38
2	A	101	OHT	C21-C20	2.66	1.44	1.38
2	A	101	OHT	C3-C2	2.67	1.43	1.38
2	A	103	OHT	C3-C4	2.73	1.44	1.38
2	B	104	OHT	C22-C21	2.74	1.43	1.38
2	B	102	OHT	C14-C15	2.82	1.45	1.38
2	B	104	OHT	C14-C15	2.86	1.45	1.38
2	A	103	OHT	C14-C15	2.87	1.45	1.38
2	A	103	OHT	C5-C4	2.89	1.44	1.38
2	A	101	OHT	C14-C15	2.90	1.45	1.38
2	B	104	OHT	C13-C14	2.91	1.45	1.38
2	B	102	OHT	C3-C2	2.95	1.44	1.38
2	B	102	OHT	C19-C18	2.95	1.44	1.38
2	B	102	OHT	C13-C14	2.97	1.45	1.38
2	A	103	OHT	C22-C21	3.00	1.44	1.38
2	B	102	OHT	C15-C16	3.07	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	OHT	C15-C16	3.10	1.45	1.38
2	B	102	OHT	C22-C21	3.15	1.44	1.38
2	A	101	OHT	C5-C4	3.19	1.45	1.38
2	A	103	OHT	C15-C16	3.21	1.45	1.38
2	A	101	OHT	C13-C14	3.25	1.46	1.38
2	B	104	OHT	C13-C12	3.26	1.45	1.38
2	B	104	OHT	C15-C16	3.28	1.45	1.38
2	A	103	OHT	C3-C2	3.30	1.44	1.38
2	B	102	OHT	C17-C7	3.33	1.54	1.49
2	A	103	OHT	C13-C12	3.34	1.45	1.38
2	B	104	OHT	C3-C2	3.35	1.44	1.38
2	A	101	OHT	C6-C5	3.38	1.44	1.38
2	B	104	OHT	C5-C4	3.43	1.45	1.38
2	A	101	OHT	C22-C21	3.49	1.45	1.38
2	A	103	OHT	C6-C5	3.50	1.45	1.38
2	B	104	OHT	C17-C7	3.52	1.55	1.49
2	B	102	OHT	C13-C12	3.60	1.46	1.38
2	B	104	OHT	C6-C5	3.61	1.45	1.38
2	A	101	OHT	C19-C18	3.62	1.45	1.38
2	B	104	OHT	C19-C18	3.72	1.45	1.38
2	A	101	OHT	C13-C12	3.73	1.46	1.38
2	A	103	OHT	C19-C18	3.73	1.45	1.38
2	B	102	OHT	C5-C4	3.73	1.46	1.38
2	A	101	OHT	C17-C7	3.77	1.55	1.49
2	B	102	OHT	C6-C5	3.80	1.45	1.38
2	B	104	OHT	C22-C17	3.98	1.46	1.39
2	A	103	OHT	C17-C7	4.25	1.56	1.49
2	B	102	OHT	C22-C17	4.37	1.46	1.39
2	A	103	OHT	C22-C17	4.41	1.46	1.39
2	B	102	OHT	C2-C1	4.43	1.46	1.39
2	A	101	OHT	C2-C1	4.48	1.47	1.39
2	A	101	OHT	C7-C8	4.52	1.47	1.34
2	A	103	OHT	C2-C1	4.55	1.47	1.39
2	B	104	OHT	C7-C8	4.63	1.47	1.34
2	B	104	OHT	C16-C11	4.63	1.47	1.39
2	B	102	OHT	C16-C11	4.67	1.47	1.39
2	B	104	OHT	C12-C11	4.75	1.47	1.39
2	A	103	OHT	C12-C11	4.77	1.47	1.39
2	A	103	OHT	C7-C8	4.78	1.48	1.34
2	A	101	OHT	C22-C17	4.79	1.47	1.39
2	B	104	OHT	C2-C1	4.84	1.47	1.39
2	B	102	OHT	C18-C17	4.86	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	OHT	C12-C11	4.87	1.47	1.39
2	A	103	OHT	C16-C11	4.90	1.47	1.39
2	B	102	OHT	C19-C20	4.91	1.48	1.38
2	A	101	OHT	C12-C11	4.92	1.47	1.39
2	B	102	OHT	C7-C8	4.96	1.48	1.34
2	A	101	OHT	C19-C20	5.02	1.48	1.38
2	A	101	OHT	C16-C11	5.18	1.48	1.39
2	A	101	OHT	C18-C17	5.20	1.48	1.39
2	A	103	OHT	C19-C20	5.24	1.49	1.38
2	B	104	OHT	C19-C20	5.26	1.49	1.38
2	A	103	OHT	C18-C17	5.27	1.48	1.39
2	B	104	OHT	C18-C17	5.30	1.48	1.39
2	A	101	OHT	C6-C1	5.40	1.48	1.39
2	A	101	OHT	C1-C7	5.64	1.58	1.49
2	A	103	OHT	C6-C1	5.77	1.49	1.39
2	B	104	OHT	C6-C1	6.01	1.49	1.39
2	B	102	OHT	C1-C7	6.25	1.59	1.49
2	B	102	OHT	C6-C1	6.50	1.50	1.39
2	B	104	OHT	C1-C7	6.53	1.60	1.49
2	A	103	OHT	C1-C7	6.62	1.60	1.49

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	OHT	C9-C8-C11	-4.84	107.35	114.39
2	A	101	OHT	C9-C8-C11	-4.57	107.74	114.39
2	B	104	OHT	C9-C8-C11	-4.34	108.07	114.39
2	A	103	OHT	C9-C8-C11	-3.96	108.63	114.39
2	B	104	OHT	C17-C7-C8	-3.60	118.02	122.84
2	A	103	OHT	C17-C7-C8	-3.55	118.08	122.84
2	A	101	OHT	C17-C7-C8	-3.33	118.37	122.84
2	B	102	OHT	C17-C7-C8	-2.54	119.44	122.84
2	A	103	OHT	C6-C1-C2	-2.49	114.90	118.60
2	B	104	OHT	C6-C1-C2	-2.39	115.05	118.60
2	A	101	OHT	C23-C24-N24	-2.31	108.29	114.66
2	A	101	OHT	C6-C1-C2	-2.22	115.30	118.60
2	B	102	OHT	C6-C1-C2	-2.10	115.48	118.60
2	B	102	OHT	C23-C24-N24	-2.01	109.12	114.66
2	B	104	OHT	C11-C8-C7	2.01	124.99	122.40
2	B	104	OHT	C23-O20-C20	2.04	122.93	117.91
2	A	103	OHT	C1-C7-C8	2.26	125.86	122.84
2	B	102	OHT	C11-C8-C7	2.34	125.43	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	103	OHT	C3-C2-C1	2.45	123.60	120.76
2	B	104	OHT	C3-C2-C1	2.57	123.74	120.76
2	A	101	OHT	C3-C2-C1	2.58	123.75	120.76
2	B	102	OHT	C3-C2-C1	2.62	123.80	120.76
2	B	104	OHT	C1-C7-C8	2.68	126.42	122.84
2	B	104	OHT	C9-C8-C7	3.04	126.93	123.47
2	A	103	OHT	C9-C8-C7	3.10	127.00	123.47
2	B	102	OHT	C1-C7-C8	3.22	127.15	122.84
2	B	102	OHT	C9-C8-C7	3.29	127.21	123.47
2	A	101	OHT	C9-C8-C7	3.78	127.77	123.47
2	A	101	OHT	C1-C7-C8	3.81	127.94	122.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	OHT	1	0
2	B	102	OHT	2	0
2	B	104	OHT	1	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 ⓘ

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	223/246 (90%)	0.41	20 (8%) 12 11	21, 38, 66, 81	0
1	B	227/246 (92%)	0.39	17 (7%) 17 17	23, 37, 70, 75	0
All	All	450/492 (91%)	0.40	37 (8%) 14 14	21, 37, 68, 81	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	260	LEU	6.5
1	B	288	PRO	6.1
1	A	426	LEU	4.7
1	A	292	ALA	4.7
1	B	290	THR	4.4
1	B	370	VAL	3.9
1	B	410	MET	3.9
1	A	424	ARG	3.8
1	A	409	SER	3.7
1	B	286	SER	3.5
1	A	425	LYS	3.5
1	B	492	LEU	3.3
1	B	495	LEU	3.3
1	B	498	HIS	3.3
1	A	370	VAL	3.2
1	B	287	ALA	3.2
1	A	371	GLU	3.1
1	A	288	PRO	3.0
1	B	278	PRO	3.0
1	B	444	SER	3.0
1	A	498	HIS	2.9
1	A	495	LEU	2.9
1	A	484	VAL	2.9
1	A	410	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	285	PRO	2.8
1	A	286	SER	2.8
1	B	369	SER	2.7
1	B	291	GLU	2.4
1	A	428	HIS	2.4
1	A	499	VAL	2.3
1	A	445	GLY	2.3
1	B	371	GLU	2.2
1	A	444	SER	2.2
1	A	449	GLN	2.1
1	B	285	PRO	2.1
1	B	409	SER	2.1
1	A	450	GLN	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	OHT	A	101	29/29	0.88	0.21	2.44	30,35,38,41	0
2	OHT	B	102	29/29	0.90	0.20	2.07	27,33,38,39	0
2	OHT	B	104	29/29	0.84	0.20	0.77	43,48,57,58	0
2	OHT	A	103	29/29	0.92	0.16	0.32	35,38,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.