



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:29 am GMT

PDB ID : 2IOK
Title : Human estrogen receptor alpha ligand-binding domain in complex with compound 1D
Authors : Fitzgerald, P.M.D.; Sharma, N.
Deposited on : 2006-10-10
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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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

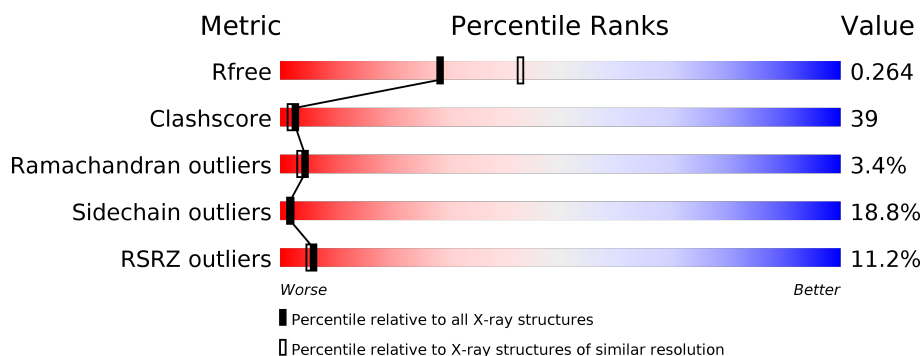
1 Overall quality at a glance

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	254	<div> <div>11%</div> <div>26% 49% 15% 11%</div> </div>
1	B	254	<div> <div>9%</div> <div>30% 48% 11% 10%</div> </div>

2 Entry composition [i](#)

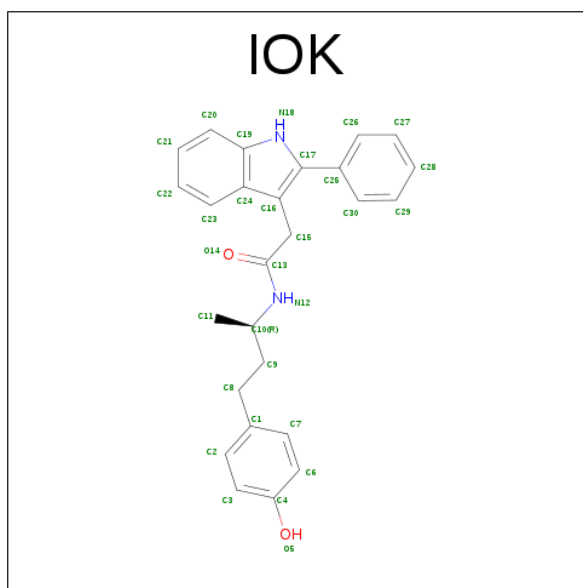
There are 3 unique types of molecules in this entry. The entry contains 3749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	227	Total	C	N	O	S	0	0	0
			1807	1162	303	324	18			
1	B	228	Total	C	N	O	S	0	0	0
			1811	1164	304	326	17			

- Molecule 2 is N-[(1R)-3-(4-HYDROXYPHENYL)-1-METHYLPROPYL]-2-(2-PHENYL-1H-INDOL-3-YL)ACETAMIDE (three-letter code: IOK) (formula: C₂₆H₂₆N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	26	2	2		
2	B	1	Total	C	N	O	0	0
			30	26	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	B	41	Total 41	O 41	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	99.86Å 99.86Å 54.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 54.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.40) 96.5 (54.90-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.39Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.215 , 0.323 0.184 , 0.264	Depositor DCC
R_{free} test set	1151 reflections (5.90%)	DCC
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.865	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.316 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3749	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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](#)

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

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	0.31	0/1838	0.76	1/2481 (0.0%)
1	B	0.30	0/1843	0.74	0/2491
All	All	0.30	0/3681	0.75	1/4972 (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	383	TRP	CA-CB-CG	5.39	123.94	113.70

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	1807	0	1852	172	0
1	B	1811	0	1853	130	0
2	A	30	0	25	5	0
2	B	30	0	25	4	0
3	A	30	0	0	2	0
3	B	41	0	0	5	0
All	All	3749	0	3755	292	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 39.

All (292) 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:496:THR:H	1:A:499:GLN:HE21	1.10	1.00
1:B:1371:THR:HG22	1:B:1373:HIS:H	1.30	0.94
1:A:371:THR:HG22	1:A:373:HIS:H	1.39	0.88
1:B:1394:ARG:HB2	1:B:1403:LEU:HD23	1.59	0.84
1:A:306:LEU:HD11	1:A:308:LEU:HD12	1.58	0.84
1:A:535:PRO:HD2	1:A:538:ASP:OD2	1.79	0.83
1:B:1418:VAL:HB	1:B:1421:MET:HG3	1.61	0.83
1:B:1312:ALA:O	1:B:1316:VAL:HG23	1.81	0.80
1:A:306:LEU:HG	1:A:308:LEU:H	1.46	0.79
1:B:1306:LEU:HD11	1:B:1308:LEU:HD12	1.64	0.79
1:A:342:MET:HE3	1:A:346:LEU:HD11	1.64	0.79
1:A:341:SER:O	1:A:345:LEU:HB2	1.83	0.79
1:A:418:VAL:HB	1:A:421:MET:HG3	1.63	0.79
1:B:1498:GLN:O	1:B:1502:GLN:HG3	1.83	0.79
1:B:1473:ASP:O	1:B:1477:ARG:HG3	1.84	0.77
1:A:411:ASP:H	1:A:414:GLN:HG3	1.48	0.77
1:A:423:GLU:O	1:A:427:MET:HG3	1.86	0.76
1:A:513:HIS:O	1:A:517:MET:HG3	1.86	0.75
1:A:502:GLN:O	1:A:506:GLN:HG3	1.87	0.75
1:B:1404:PHE:HE1	1:B:1410:LEU:HD12	1.50	0.74
1:A:409:LEU:O	1:A:410:LEU:HD23	1.88	0.74
1:A:524:HIS:HA	1:A:527:SER:HB3	1.68	0.74
1:A:307:ALA:O	1:A:481:LYS:HD3	1.87	0.74
1:A:312:ALA:O	1:A:316:VAL:HG23	1.86	0.73
1:A:330:GLU:HG3	1:A:352:ARG:NH1	2.03	0.73
1:B:1463:SER:HB3	1:B:1465:THR:HG23	1.69	0.73
1:A:433:SER:O	1:A:437:MET:HG3	1.87	0.73
1:A:496:THR:OG1	1:A:499:GLN:HG3	1.89	0.73
1:A:316:VAL:HG12	1:A:320:LEU:HD11	1.72	0.72
1:B:1423:GLU:O	1:B:1427:MET:HG3	1.89	0.72
1:A:497:LEU:HD22	1:B:1497:LEU:HD22	1.72	0.71
1:A:421:MET:HE2	1:A:425:PHE:HE1	1.55	0.71
1:B:1371:THR:HG22	1:B:1373:HIS:N	2.04	0.70
1:A:519:ASN:O	1:A:523:GLU:HG3	1.91	0.69
1:A:367:PHE:HE1	1:A:378:LEU:HD12	1.56	0.69
1:B:1382:ALA:HB2	1:B:1456:SER:HB2	1.75	0.69
1:A:434:ARG:NH1	1:A:438:MET:HG2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1415:GLY:O	1:B:1421:MET:HB2	1.92	0.69
1:A:467:LYS:HA	1:A:470:GLU:OE1	1.93	0.69
1:A:464:SER:OG	1:A:469:LEU:HD12	1.94	0.68
1:B:1454:LEU:O	1:B:1458:VAL:HG22	1.93	0.68
1:A:539:LEU:O	1:A:543:MET:HG3	1.94	0.67
1:A:495:LEU:HB3	1:A:499:GLN:HB2	1.77	0.67
1:B:1351:ASP:O	1:B:1354:LEU:HB2	1.94	0.67
1:B:1376:VAL:O	1:B:1380:GLU:HB2	1.96	0.66
1:B:1474:HIS:O	1:B:1478:VAL:HG23	1.94	0.66
1:A:306:LEU:HD21	1:A:308:LEU:HB2	1.76	0.66
1:A:331:TYR:OH	1:A:407:ASN:HB2	1.96	0.66
1:A:434:ARG:O	1:A:438:MET:HG3	1.97	0.65
1:B:1502:GLN:O	1:B:1506:GLN:HG3	1.97	0.65
1:B:1424:ILE:HA	1:B:1427:MET:HE2	1.78	0.64
1:A:496:THR:H	1:A:499:GLN:NE2	1.91	0.64
1:B:1379:LEU:HD12	1:B:1544:LEU:HD11	1.78	0.64
1:B:1524:HIS:HA	1:B:1527:SER:HB3	1.78	0.64
1:B:1404:PHE:CE1	1:B:1410:LEU:HD12	2.33	0.64
1:A:498:GLN:O	1:A:502:GLN:HG3	1.97	0.64
1:A:315:MET:HE1	1:A:481:LYS:HG2	1.80	0.63
1:B:1325:PRO:HG2	1:B:1327:LEU:HD21	1.79	0.63
1:B:1498:GLN:HE21	1:B:1502:GLN:NE2	1.97	0.63
1:A:519:ASN:HD22	1:B:1519:ASN:HD22	1.45	0.63
1:A:410:LEU:HA	1:A:414:GLN:OE1	1.99	0.63
1:A:377:HIS:HE2	1:A:457:GLY:HA3	1.63	0.62
1:A:421:MET:HE2	1:A:425:PHE:CE1	2.33	0.62
1:B:1382:ALA:O	1:B:1386:ILE:HD12	1.99	0.61
1:A:473:ASP:O	1:A:477:ARG:HG3	2.01	0.61
1:B:1401:LYS:HD3	1:B:1409:LEU:HG	1.82	0.61
1:A:323:GLU:OE2	1:A:446:VAL:HG12	2.01	0.61
1:B:1503:ARG:HA	1:B:1506:GLN:NE2	2.16	0.60
1:A:342:MET:HB3	1:A:418:VAL:HG21	1.83	0.60
1:B:1440:LEU:HD12	1:B:1444:GLU:OE1	2.02	0.60
1:A:382:ALA:O	1:A:386:ILE:HD12	2.02	0.59
1:A:502:GLN:OE1	1:B:1480:ASP:HB3	2.01	0.59
2:A:600:IOK:H151	2:A:600:IOK:H26	1.83	0.59
1:B:1310:LEU:O	1:B:1481:LYS:HE2	2.03	0.59
1:A:374:ASP:O	1:A:378:LEU:HG	2.03	0.58
1:A:403:LEU:HD11	1:A:406:PRO:HA	1.85	0.58
1:B:1372:LEU:O	1:B:1376:VAL:HG23	2.03	0.58
1:A:367:PHE:CE1	1:A:378:LEU:HD12	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ASN:O	1:A:363:ARG:HG3	2.04	0.57
1:B:1389:ILE:O	1:B:1445:PHE:HE1	1.88	0.57
1:A:311:THR:HB	1:A:314:GLN:HG3	1.86	0.57
1:B:1468:SER:O	1:B:1472:LYS:HG3	2.05	0.57
1:B:1306:LEU:HD11	1:B:1308:LEU:CD1	2.34	0.57
1:B:1323:GLU:OE2	1:B:1446:VAL:HG12	2.04	0.57
1:B:1358:ILE:HD13	1:B:1543:MET:HE2	1.87	0.57
1:A:377:HIS:NE2	1:A:457:GLY:HA3	2.20	0.56
1:A:484:ASP:OD2	1:B:1498:GLN:HG3	2.05	0.56
1:B:1359:ASN:O	1:B:1363:ARG:HG3	2.05	0.56
1:A:316:VAL:HG12	1:A:320:LEU:CD1	2.35	0.56
1:A:536:LEU:HD11	1:A:540:LEU:HD21	1.88	0.56
1:B:1382:ALA:HB2	1:B:1456:SER:CB	2.36	0.56
1:A:497:LEU:HD22	1:B:1497:LEU:CD2	2.34	0.56
1:A:376:VAL:O	1:A:380:GLU:HB2	2.06	0.56
1:A:461:PHE:CD2	1:A:472:LYS:HE2	2.41	0.56
1:B:1401:LYS:HA	1:B:1410:LEU:O	2.06	0.56
1:A:519:ASN:ND2	1:B:1519:ASN:HD22	2.04	0.56
1:A:524:HIS:CA	1:A:527:SER:HB3	2.34	0.55
1:A:444:GLU:HG2	1:A:486:LEU:HD23	1.88	0.55
1:B:1498:GLN:HE21	1:B:1502:GLN:HE22	1.53	0.55
1:B:1514:ILE:HA	1:B:1517:MET:HE3	1.88	0.55
1:A:454:LEU:O	1:A:458:VAL:HG22	2.06	0.55
1:A:421:MET:O	1:A:425:PHE:HB2	2.07	0.55
1:A:318:ALA:HA	1:A:321:ASP:HB2	1.88	0.55
1:A:342:MET:SD	1:A:346:LEU:HG	2.47	0.55
1:B:1435:PHE:CE1	1:B:1510:ILE:HD13	2.42	0.55
1:A:410:LEU:HD13	1:A:414:GLN:HB3	1.88	0.54
1:A:311:THR:H	1:A:314:GLN:HB2	1.73	0.54
1:B:1505:ALA:O	1:B:1509:LEU:HG	2.07	0.54
1:A:410:LEU:HD13	1:A:414:GLN:CB	2.38	0.54
1:A:486:LEU:O	1:A:489:LEU:HB2	2.08	0.54
1:B:1341:SER:O	1:B:1345:LEU:HB2	2.08	0.54
1:A:458:VAL:HG11	1:A:476:HIS:CE1	2.43	0.54
1:B:1463:SER:CB	1:B:1465:THR:HG23	2.38	0.54
1:A:351:ASP:O	1:A:354:LEU:HB2	2.08	0.53
1:A:524:HIS:CD2	2:A:600:IOK:H27	2.43	0.53
1:B:1316:VAL:O	1:B:1319:LEU:HB2	2.09	0.53
1:A:306:LEU:HG	1:A:308:LEU:N	2.19	0.53
1:A:490:MET:O	1:A:493:ALA:HB3	2.08	0.53
1:B:1306:LEU:HG	1:B:1308:LEU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:TYR:HB2	1:B:1513:HIS:CE1	2.44	0.53
1:A:342:MET:HB3	1:A:418:VAL:CG2	2.39	0.52
1:A:450:SER:O	1:A:453:LEU:HB3	2.09	0.52
1:B:1467:LYS:HA	1:B:1470:GLU:OE1	2.08	0.52
1:B:1334:THR:O	1:B:1334:THR:HG22	2.10	0.52
1:A:364:VAL:HG21	1:A:453:LEU:HD23	1.91	0.52
1:A:361:ALA:HB2	1:A:379:LEU:HD21	1.92	0.52
1:A:435:PHE:CD1	1:A:440:LEU:HD22	2.44	0.52
1:A:364:VAL:HG21	1:A:453:LEU:CD2	2.40	0.52
1:B:1377:HIS:NE2	1:B:1457:GLY:HA3	2.25	0.52
1:A:403:LEU:HD13	1:A:409:LEU:HD13	1.90	0.51
1:B:1482:ILE:O	1:B:1485:THR:HB	2.10	0.51
1:A:320:LEU:HD21	1:A:443:GLU:HG3	1.91	0.51
1:B:1370:LEU:HB2	1:B:1375:GLN:HE21	1.76	0.51
1:B:1496:THR:OG1	1:B:1499:GLN:OE1	2.26	0.51
1:A:311:THR:CB	1:A:314:GLN:HG3	2.40	0.51
1:A:361:ALA:CB	1:A:379:LEU:HD21	2.40	0.51
1:B:1480:ASP:O	1:B:1484:ASP:OD1	2.29	0.51
1:A:411:ASP:N	1:A:414:GLN:HG3	2.21	0.50
1:A:306:LEU:HD11	1:A:308:LEU:CD1	2.34	0.50
1:B:1311:THR:OG1	1:B:1314:GLN:OE1	2.30	0.50
1:B:1401:LYS:HB3	1:B:1409:LEU:HG	1.92	0.50
1:A:466:LEU:O	1:A:470:GLU:OE1	2.28	0.50
1:A:353:GLU:OE1	2:A:600:IOK:O5	2.30	0.50
1:A:482:ILE:O	1:A:485:THR:HB	2.12	0.50
1:A:448:LEU:HD11	1:A:507:LEU:HD22	1.94	0.50
1:A:464:SER:O	1:A:465:THR:O	2.30	0.49
1:B:1519:ASN:O	1:B:1523:GLU:HG3	2.12	0.49
1:A:454:LEU:HB2	1:A:479:LEU:HD21	1.95	0.49
1:B:1435:PHE:CD1	1:B:1440:LEU:HD22	2.47	0.49
1:B:1436:ARG:HD2	3:B:1611:HOH:O	2.12	0.49
1:B:1353:GLU:OE1	2:B:1600:IOK:O5	2.30	0.49
1:A:315:MET:CE	1:A:481:LYS:HG2	2.41	0.49
1:A:328:TYR:HA	1:A:405:ALA:HB1	1.94	0.49
1:B:1331:TYR:HA	3:B:1639:HOH:O	2.13	0.49
1:B:1384:LEU:HB2	1:B:1522:MET:HE1	1.94	0.49
1:A:480:ASP:O	1:A:484:ASP:OD1	2.31	0.49
1:B:1425:PHE:O	1:B:1428:LEU:HB2	2.13	0.49
1:B:1399:PRO:HA	1:B:1436:ARG:HH22	1.77	0.49
1:A:524:HIS:O	1:A:527:SER:HB3	2.11	0.49
1:B:1343:MET:O	1:B:1346:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LEU:O	1:A:544:LEU:HB2	2.13	0.48
1:A:328:TYR:CE2	1:A:406:PRO:HB2	2.49	0.48
1:A:460:THR:O	1:A:460:THR:HG22	2.13	0.48
1:A:368:VAL:HA	1:A:375:GLN:NE2	2.29	0.48
1:A:402:LEU:HD12	1:A:425:PHE:CE2	2.49	0.48
1:A:317:SER:O	1:A:321:ASP:HB2	2.14	0.48
1:B:1331:TYR:O	1:B:1333:PRO:HD3	2.13	0.48
1:A:519:ASN:HD22	1:B:1519:ASN:ND2	2.09	0.48
1:B:1311:THR:H	1:B:1314:GLN:HB2	1.79	0.48
1:B:1478:VAL:O	1:B:1482:ILE:HG13	2.14	0.48
2:B:1600:IOK:H151	2:B:1600:IOK:H26	1.95	0.48
1:A:415:GLY:O	1:A:421:MET:HB2	2.14	0.47
1:B:1459:TYR:O	1:B:1460:THR:OG1	2.29	0.47
1:A:388:MET:HE3	1:A:518:SER:HA	1.97	0.47
1:A:311:THR:HG1	1:A:314:GLN:CD	2.17	0.47
1:B:1523:GLU:HA	3:B:1630:HOH:O	2.14	0.47
1:B:1490:MET:SD	1:B:1503:ARG:HG2	2.55	0.47
1:B:1448:LEU:O	1:B:1452:ILE:HG13	2.14	0.47
1:A:308:LEU:HA	1:A:481:LYS:HD3	1.97	0.46
1:B:1426:ASP:HB3	3:B:1623:HOH:O	2.15	0.46
1:A:343:MET:SD	2:A:600:IOK:H30	2.56	0.46
1:A:384:LEU:O	1:A:388:MET:HG3	2.15	0.46
1:A:401:LYS:HB3	1:A:410:LEU:O	2.16	0.46
1:B:1503:ARG:HA	1:B:1506:GLN:HE21	1.80	0.46
1:A:311:THR:HG22	1:A:312:ALA:H	1.81	0.46
1:A:449:LYS:HB3	1:A:449:LYS:HE3	1.66	0.46
1:B:1399:PRO:HG3	1:B:1436:ARG:CZ	2.46	0.46
1:A:330:GLU:HG3	1:A:352:ARG:HH12	1.78	0.45
1:B:1464:SER:O	1:B:1465:THR:O	2.34	0.45
1:B:1377:HIS:NE2	1:B:1457:GLY:O	2.50	0.45
1:A:399:PRO:HA	1:A:436:ARG:HH22	1.80	0.45
1:B:1418:VAL:HG12	1:B:1419:GLU:N	2.32	0.45
1:A:343:MET:HE1	1:A:418:VAL:HG11	1.98	0.45
1:A:352:ARG:HG3	1:A:352:ARG:H	1.41	0.45
1:B:1367:PHE:O	1:B:1375:GLN:NE2	2.49	0.45
1:B:1535:PRO:HD2	1:B:1538:ASP:HB2	1.99	0.45
1:A:459:TYR:HA	1:A:472:LYS:NZ	2.32	0.45
1:A:344:GLY:O	1:A:348:ASN:HB2	2.17	0.45
1:A:444:GLU:OE1	1:A:503:ARG:NH2	2.49	0.45
1:A:475:ILE:HG22	1:A:476:HIS:N	2.32	0.45
1:A:308:LEU:HD11	1:A:474:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1326:ILE:N	1:B:1326:ILE:HD13	2.31	0.45
1:B:1330:GLU:OE2	1:B:1352:ARG:NH1	2.50	0.45
1:A:343:MET:O	1:A:346:LEU:N	2.49	0.44
1:A:535:PRO:N	3:A:614:HOH:O	2.50	0.44
1:B:1377:HIS:HE2	1:B:1457:GLY:HA3	1.82	0.44
1:B:1484:ASP:O	1:B:1488:HIS:HB3	2.17	0.44
1:B:1525:LEU:HD21	2:B:1600:IOK:C19	2.47	0.44
1:A:469:LEU:O	1:A:473:ASP:HB3	2.17	0.44
1:A:483:THR:HG21	1:B:1502:GLN:HA	1.99	0.44
1:B:1450:SER:O	1:B:1453:LEU:HB3	2.17	0.44
1:A:396:MET:O	1:A:436:ARG:NE	2.50	0.44
1:A:410:LEU:HD22	1:A:414:GLN:CD	2.38	0.44
1:A:377:HIS:HE2	1:A:457:GLY:CA	2.28	0.44
1:A:508:LEU:HD22	1:B:1509:LEU:HD21	1.99	0.44
1:A:313:ASP:N	1:A:313:ASP:OD1	2.50	0.44
1:A:323:GLU:HA	1:A:324:PRO:HD3	1.77	0.44
1:A:424:ILE:HD11	1:A:524:HIS:CD2	2.53	0.44
1:A:457:GLY:HA2	3:A:608:HOH:O	2.18	0.44
1:B:1342:MET:HB3	1:B:1418:VAL:CG2	2.48	0.44
1:A:372:LEU:O	1:A:376:VAL:HG23	2.18	0.43
1:B:1540:LEU:O	1:B:1544:LEU:HB2	2.18	0.43
1:A:509:LEU:HD21	1:B:1511:LEU:HD12	2.00	0.43
1:B:1325:PRO:HG2	1:B:1327:LEU:CD2	2.45	0.43
1:B:1354:LEU:HD23	1:B:1357:MET:CE	2.48	0.43
1:B:1525:LEU:HD23	1:B:1525:LEU:HA	1.72	0.43
1:B:1536:LEU:O	1:B:1540:LEU:HG	2.18	0.43
1:A:311:THR:OG1	1:A:314:GLN:OE1	2.26	0.43
1:A:371:THR:HG22	1:A:373:HIS:N	2.21	0.43
1:A:396:MET:CE	1:A:436:ARG:HA	2.48	0.43
1:A:358:ILE:HG21	1:A:543:MET:HE2	2.00	0.43
1:A:394:ARG:NH2	1:A:404:PHE:O	2.50	0.43
1:A:459:TYR:HD2	1:B:1513:HIS:ND1	2.17	0.43
1:B:1380:GLU:OE1	1:B:1537:TYR:HD2	2.01	0.43
1:B:1541:LEU:HD23	1:B:1541:LEU:HA	1.84	0.43
2:B:1600:IOK:H91	2:B:1600:IOK:H7	1.82	0.43
1:A:329:SER:OG	1:A:330:GLU:N	2.52	0.43
1:A:458:VAL:O	1:A:472:LYS:NZ	2.50	0.43
1:A:536:LEU:CD1	1:A:540:LEU:HD21	2.48	0.42
1:B:1457:GLY:HA2	3:B:1607:HOH:O	2.19	0.42
1:A:342:MET:O	1:A:346:LEU:HG	2.20	0.42
1:A:421:MET:HE2	1:A:421:MET:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ASN:OD1	1:B:1509:LEU:HB3	2.19	0.42
1:A:506:GLN:HG3	1:A:506:GLN:H	1.71	0.42
1:A:543:MET:HB3	1:A:543:MET:HE3	1.82	0.42
1:B:1391:LEU:HD13	1:B:1404:PHE:CD2	2.54	0.42
1:B:1467:LYS:HD2	1:B:1467:LYS:HA	1.58	0.42
1:A:316:VAL:O	1:A:320:LEU:HG	2.19	0.42
1:B:1318:ALA:HA	1:B:1321:ASP:HB2	2.01	0.42
1:B:1433:SER:O	1:B:1437:MET:HG3	2.19	0.42
1:A:478:VAL:O	1:A:481:LYS:HB3	2.20	0.42
1:A:496:THR:O	1:A:499:GLN:N	2.52	0.42
1:B:1455:ASN:HA	1:B:1458:VAL:CG2	2.50	0.42
1:A:316:VAL:HG11	1:A:443:GLU:HG2	2.01	0.42
1:B:1372:LEU:HD21	1:B:1541:LEU:HD22	2.01	0.42
1:B:1418:VAL:CB	1:B:1421:MET:HG3	2.40	0.42
1:A:427:MET:HB3	1:A:513:HIS:NE2	2.35	0.42
1:A:459:TYR:HB2	1:B:1513:HIS:HE1	1.82	0.42
1:B:1313:ASP:OD1	1:B:1313:ASP:N	2.50	0.42
1:B:1331:TYR:HE1	1:B:1407:ASN:O	2.03	0.42
1:A:412:ARG:O	1:A:416:LYS:N	2.53	0.41
1:A:495:LEU:HB3	1:A:499:GLN:CB	2.47	0.41
1:B:1398:HIS:N	1:B:1399:PRO:HD3	2.33	0.41
1:B:1486:LEU:O	1:B:1490:MET:HG3	2.20	0.41
1:A:408:LEU:CD1	1:A:410:LEU:HD21	2.50	0.41
1:A:422:VAL:HG13	1:A:423:GLU:N	2.36	0.41
1:B:1422:VAL:HG13	1:B:1423:GLU:N	2.34	0.41
1:B:1388:MET:HG2	1:B:1428:LEU:HD21	2.02	0.41
1:A:350:ALA:O	1:A:353:GLU:N	2.50	0.41
1:A:447:CYS:HB3	1:A:486:LEU:HD11	2.03	0.41
1:B:1315:MET:HE2	1:B:1315:MET:HB2	1.96	0.41
1:B:1373:HIS:ND1	1:B:1537:TYR:OH	2.54	0.41
1:A:319:LEU:HA	1:A:319:LEU:HD23	1.95	0.41
1:A:343:MET:O	1:A:346:LEU:HB2	2.21	0.41
1:A:363:ARG:HB3	1:A:363:ARG:HE	1.40	0.41
1:A:308:LEU:HA	1:A:481:LYS:CD	2.51	0.41
1:A:535:PRO:HD2	1:A:538:ASP:CG	2.39	0.41
1:B:1354:LEU:HD23	1:B:1357:MET:HE3	2.03	0.41
1:A:411:ASP:O	1:A:414:GLN:N	2.54	0.41
1:A:418:VAL:CB	1:A:421:MET:HG3	2.42	0.41
1:A:382:ALA:HB2	1:A:456:SER:HB2	2.03	0.40
1:A:435:PHE:CG	1:A:440:LEU:HD22	2.56	0.40
1:A:397:GLU:C	1:A:399:PRO:HD3	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:600:IOK:C23	2:A:600:IOK:H81	2.52	0.40
1:B:1370:LEU:HB3	1:B:1371:THR:H	1.62	0.40
1:B:1460:THR:O	1:B:1460:THR:HG22	2.21	0.40
1:A:413:ASN:N	1:A:413:ASN:OD1	2.52	0.40
1:B:1307:ALA:O	1:B:1310:LEU:HB2	2.22	0.40
1:B:1403:LEU:CD1	1:B:1409:LEU:HD13	2.51	0.40
1:A:540:LEU:H	1:A:540:LEU:HG	1.74	0.40
1:B:1310:LEU:HD23	1:B:1310:LEU:HA	1.81	0.40
1:B:1465:THR:OG1	1:B:1468:SER:HB2	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	221/254 (87%)	192 (87%)	21 (10%)	8 (4%)	4	3
1	B	222/254 (87%)	191 (86%)	24 (11%)	7 (3%)	5	4
All	All	443/508 (87%)	383 (86%)	45 (10%)	15 (3%)	4	3

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	THR
1	B	1370	LEU
1	B	1418	VAL
1	B	1465	THR
1	A	370	LEU
1	A	378	LEU
1	B	1378	LEU
1	A	329	SER
1	A	461	PHE

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Mol	Chain	Res	Type
1	A	462	LEU
1	B	1412	ARG
1	B	1460	THR
1	B	1461	PHE
1	A	456	SER
1	A	458	VAL

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	202/229 (88%)	163 (81%)	39 (19%)	1	2
1	B	203/229 (89%)	166 (82%)	37 (18%)	2	2
All	All	405/458 (88%)	329 (81%)	76 (19%)	2	2

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	309	SER
1	A	313	ASP
1	A	321	ASP
1	A	324	PRO
1	A	342	MET
1	A	345	LEU
1	A	352	ARG
1	A	363	ARG
1	A	368	VAL
1	A	412	ARG
1	A	413	ASN
1	A	414	GLN
1	A	421	MET
1	A	424	ILE
1	A	425	PHE
1	A	431	THR

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Mol	Chain	Res	Type
1	A	432	SER
1	A	434	ARG
1	A	438	MET
1	A	443	GLU
1	A	449	LYS
1	A	450	SER
1	A	455	ASN
1	A	459	TYR
1	A	467	LYS
1	A	468	SER
1	A	469	LEU
1	A	481	LYS
1	A	486	LEU
1	A	497	LEU
1	A	503	ARG
1	A	506	GLN
1	A	512	SER
1	A	526	TYR
1	A	527	SER
1	A	528	MET
1	A	536	LEU
1	A	543	MET
1	B	1306	LEU
1	B	1309	SER
1	B	1311	THR
1	B	1313	ASP
1	B	1321	ASP
1	B	1341	SER
1	B	1342	MET
1	B	1345	LEU
1	B	1349	LEU
1	B	1352	ARG
1	B	1368	VAL
1	B	1414	GLN
1	B	1419	GLU
1	B	1421	MET
1	B	1423	GLU
1	B	1424	ILE
1	B	1432	SER
1	B	1434	ARG
1	B	1450	SER
1	B	1458	VAL

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Mol	Chain	Res	Type
1	B	1467	LYS
1	B	1468	SER
1	B	1469	LEU
1	B	1473	ASP
1	B	1481	LYS
1	B	1484	ASP
1	B	1487	ILE
1	B	1492	LYS
1	B	1497	LEU
1	B	1503	ARG
1	B	1506	GLN
1	B	1520	LYS
1	B	1526	TYR
1	B	1527	SER
1	B	1536	LEU
1	B	1542	GLU
1	B	1543	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	ASN
1	A	476	HIS
1	A	499	GLN
1	A	524	HIS
1	B	1359	ASN
1	B	1441	GLN
1	B	1476	HIS
1	B	1502	GLN
1	B	1519	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
2	IOK	A	600	-	32,33,33	0.88	0	38,45,45	1.28	5 (13%)
2	IOK	B	1600	-	32,33,33	0.86	0	38,45,45	1.25	5 (13%)

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	IOK	A	600	-	-	0/17/17/17	0/4/4/4
2	IOK	B	1600	-	-	0/17/17/17	0/4/4/4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1600	IOK	C9-C10-N12	-2.77	107.11	110.61
2	A	600	IOK	C30-C25-C17	-2.69	116.35	120.59
2	B	1600	IOK	C30-C25-C17	-2.51	116.64	120.59
2	A	600	IOK	C8-C9-C10	-2.24	110.47	114.01
2	B	1600	IOK	C11-C10-C9	-2.07	108.32	111.30
2	B	1600	IOK	C17-N18-C19	2.35	108.72	103.94
2	B	1600	IOK	C26-C25-C17	2.51	124.55	120.59
2	A	600	IOK	C17-N18-C19	2.55	109.12	103.94
2	A	600	IOK	C15-C13-N12	2.66	120.11	115.89
2	A	600	IOK	C26-C25-C17	2.71	124.87	120.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	IOK	5	0
2	B	1600	IOK	4	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	227/254 (89%)	0.81	27 (11%)	5 4	13, 41, 83, 104	0
1	B	228/254 (89%)	0.61	24 (10%)	7 6	14, 41, 83, 104	0
All	All	455/508 (89%)	0.71	51 (11%)	6 5	13, 41, 84, 104	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	LEU	14.2
1	A	464	SER	13.3
1	A	340	ALA	11.2
1	A	462	LEU	10.3
1	B	1340	ALA	9.0
1	A	461	PHE	7.6
1	B	1526	TYR	6.7
1	A	339	GLU	6.6
1	A	341	SER	6.0
1	A	466	LEU	5.1
1	A	463	SER	4.9
1	B	1334	THR	4.8
1	B	1457	GLY	4.8
1	B	1462	LEU	4.6
1	A	537	TYR	4.1
1	A	331	TYR	4.0
1	A	307	ALA	4.0
1	A	526	TYR	3.7
1	B	1341	SER	3.7
1	A	525	LEU	3.6
1	B	1466	LEU	3.6
1	B	1525	LEU	3.6
1	B	1461	PHE	3.4
1	A	422	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	470	GLU	3.3
1	A	418	VAL	3.3
1	A	414	GLN	3.2
1	B	1535	PRO	3.2
1	A	468	SER	3.1
1	B	1333	PRO	3.0
1	B	1543	MET	2.9
1	B	1459	TYR	2.9
1	B	1447	CYS	2.9
1	B	1469	LEU	2.8
1	B	1335	ARG	2.8
1	A	417	CYS	2.8
1	A	535	PRO	2.6
1	B	1342	MET	2.5
1	B	1539	LEU	2.4
1	B	1308	LEU	2.4
1	A	327	LEU	2.4
1	A	325	PRO	2.4
1	A	342	MET	2.4
1	B	1464	SER	2.3
1	B	1524	HIS	2.2
1	A	458	VAL	2.2
1	B	1468	SER	2.2
1	A	326	ILE	2.2
1	B	1538	ASP	2.2
1	A	312	ALA	2.2
1	B	1307	ALA	2.1

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(\AA^2)	Q<0.9
2	IOK	B	1600	30/30	0.88	0.19	0.02	16,27,41,46	0
2	IOK	A	600	30/30	0.89	0.18	-0.13	9,33,52,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.