



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:52 PM UTC

PDB ID : 2IOK / pdb_00002iok
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

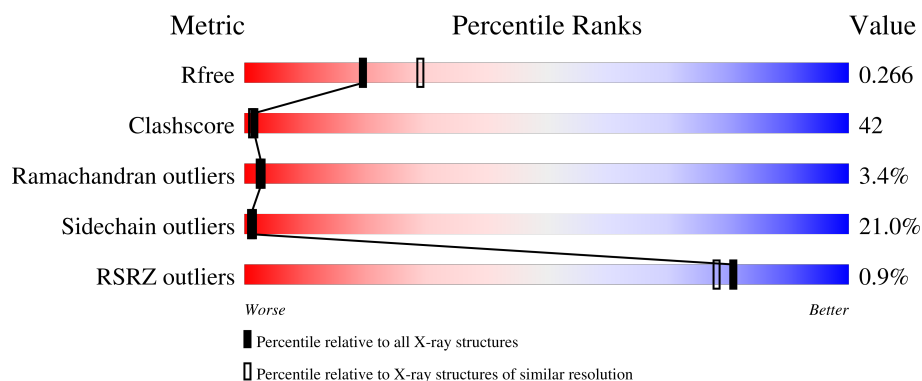
1 Overall quality at a glance

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	254	

2 Entry composition [i](#)

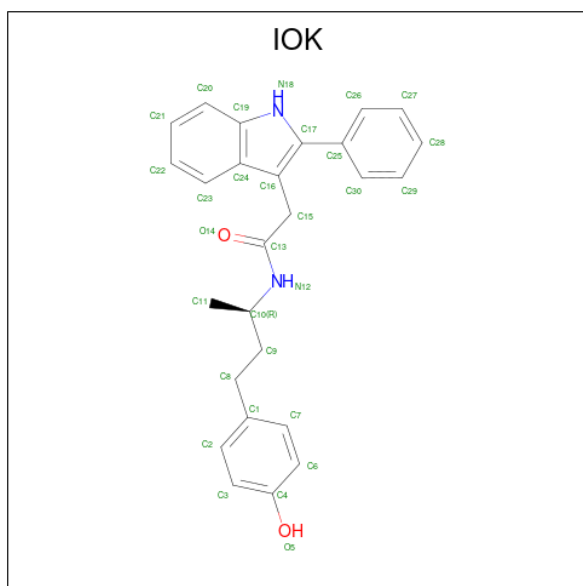
There are 3 unique types of molecules in this entry. The entry contains 3749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: IOK) (formula: $C_{26}H_{26}N_2O_2$).



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		

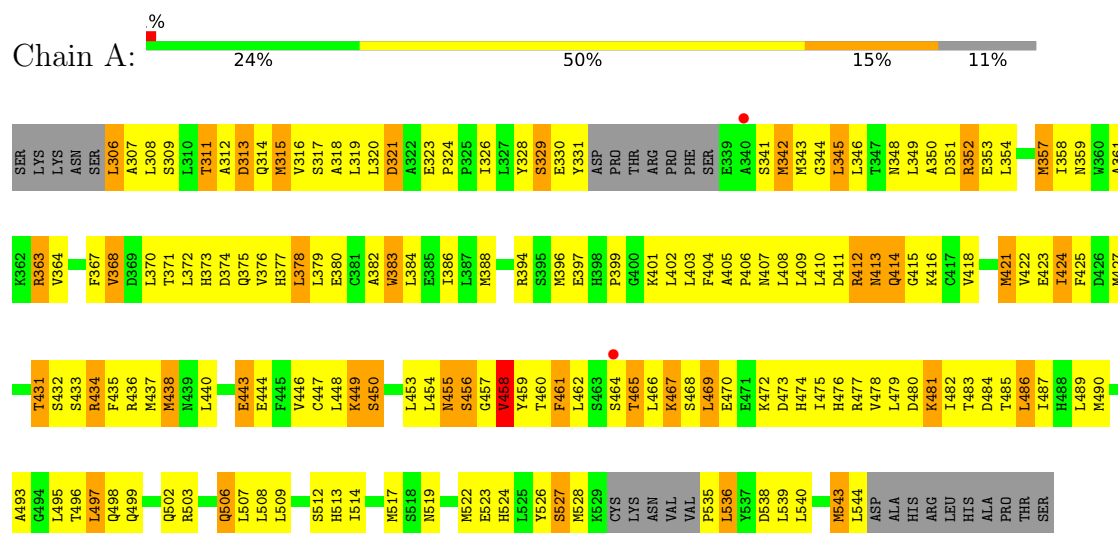
- Molecule 3 is water.

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

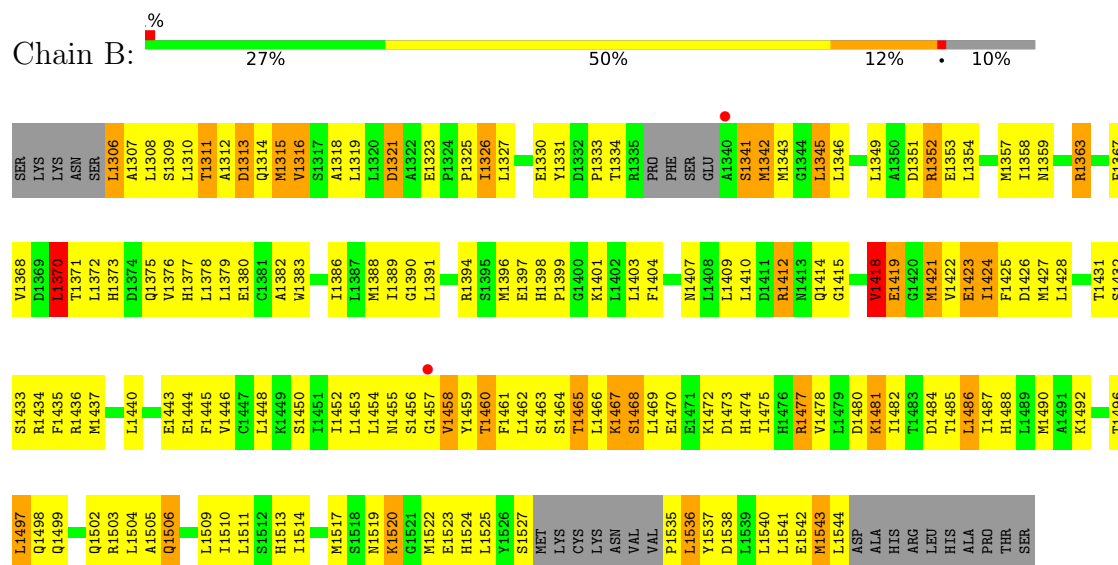
3 Residue-property plots

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

• Molecule 1: Estrogen receptor



• Molecule 1: Estrogen receptor



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 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.40) 96.4 (10.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.39Å)	Xtriage
Refinement program	SHELXL 97-1, SHELXL-97	Depositor
R, R_{free}	0.215 , 0.323 0.183 , 0.266	Depositor DCC
R_{free} test set	1198 reflections (5.59%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.856	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.316 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	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	0.37	0/1838	1.17	1/2481 (0.0%)
1	B	0.37	0/1843	1.16	7/2491 (0.3%)
All	All	0.37	0/3681	1.16	8/4972 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1370	LEU	CA-C-N	7.02	133.84	122.81
1	B	1370	LEU	C-N-CA	7.02	133.84	122.81
1	A	383	TRP	CA-CB-CG	5.44	123.94	113.60
1	B	1418	VAL	CA-C-O	-5.38	114.06	120.78
1	B	1316	VAL	CA-C-N	5.17	127.98	120.79
1	B	1316	VAL	C-N-CA	5.17	127.98	120.79
1	B	1390	GLY	CA-C-N	5.11	127.44	120.54
1	B	1390	GLY	C-N-CA	5.11	127.44	120.54

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	185	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1811	0	1853	136	0
2	A	30	0	25	8	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	311	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 42.

All (311) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1427:MET:HE1	1:B:1520:LYS:HG2	1.70	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:B:1371:THR:HG22	1:B:1373:HIS:N	2.04	0.70
1:A:343:MET:HE1	2:A:600:IOK:H29	1.73	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
1:B:1415:GLY:O	1:B:1421:MET:HB2	1.92	0.69
1:A:384:LEU:HG	1:A:388:MET:HE3	1.74	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:1354:LEU:HD23	1:B:1357:MET:HE3	1.80	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: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: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:A:396:MET:HE3	1:A:436:ARG:HA	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:342:MET:HE1	1:A:346:LEU:HD21	1.85	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:383:TRP:CZ2	1:A:522:MET:HE1	2.39	0.58
1:A:367:PHE:CE1	1:A:378:LEU:HD12	2.36	0.57
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:A:343:MET:HE1	2:A:600:IOK:C29	2.34	0.57
1:B:1468:SER:O	1:B:1472:LYS:HG3	2.05	0.57
1:A:342:MET:HE3	1:A:346:LEU:HD11	1.87	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: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:342:MET:HE2	1:A:410:LEU:HD12	1.88	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: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:B:1427:MET:HE1	1:B:1520:LYS:CG	2.35	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:THR:H	1:A:314:GLN:HB2	1.73	0.54
1:A:354:LEU:HD23	1:A:357:MET:HE3	1.89	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:421:MET:HE2	1:A:425:PHE:CE1	2.43	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:B:1424:ILE:HA	1:B:1427:MET:HE3	1.89	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:B:1396:MET:HE3	1:B:1436:ARG:HA	1.91	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
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:HG22	1:B:1334:THR:O	2.10	0.52
1:A:364:VAL:HG21	1:A:453:LEU:HD23	1.91	0.52
1:B:1383:TRP:CE2	1:B:1522:MET:HE1	2.44	0.52
1:A:361:ALA:HB2	1:A:379:LEU:HD21	1.92	0.52
1:A:311:THR:HG1	1:A:314:GLN:CD	2.17	0.52
1:A:364:VAL:HG21	1:A:453:LEU:CD2	2.40	0.52
1:A:435:PHE:CD1	1:A:440:LEU:HD22	2.44	0.52
1:A:421:MET:HE2	1:A:425:PHE:HE1	1.73	0.52
1:B:1358:ILE:HD13	1:B:1543:MET:HE2	1.92	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:A:315:MET:CE	1:A:481:LYS:HG2	2.41	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1353:GLU:OE1	2:B:1600:IOK:O5	2.30	0.49
1:B:1436:ARG:HD2	3:B:1611:HOH:O	2.12	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: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
1:A:410:LEU:HD22	1:A:414:GLN:CD	2.38	0.48
1:A:540:LEU:O	1:A:544:LEU:HB2	2.13	0.48
1:B:1514:ILE:HA	1:B:1517:MET:HE3	1.96	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:A:519:ASN:HD22	1:B:1519:ASN:ND2	2.09	0.48
1:B:1331:TYR:O	1:B:1333:PRO:HD3	2.13	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:H26	2:B:1600:IOK:H151	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:315:MET:HE2	1:A:315:MET:HB2	1.67	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:MET:HE1	1:A:481:LYS:HG2	1.96	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:A:535:PRO:HD2	1:A:538:ASP:CG	2.39	0.45
1:B:1464:SER:O	1:B:1465:THR:O	2.34	0.45
1:B:1315:MET:HE2	1:B:1315:MET:HB2	1.69	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:B:1433:SER:C	1:B:1437:MET:HE3	2.41	0.45
1:A:352:ARG:H	1:A:352:ARG:HG3	1.41	0.45
1:B:1367:PHE:O	1:B:1375:GLN:NE2	2.49	0.45
1:A:543:MET:HE3	1:A:543:MET:HB3	1.79	0.45
1:B:1535:PRO:HD2	1:B:1538:ASP:HB2	1.99	0.45
1:A:397:GLU:C	1:A:399:PRO:HD3	2.42	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
1:B:1326:ILE:HD13	1:B:1326:ILE:N	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:434:ARG:HA	1:A:437:MET:HE3	2.00	0.44
1:A:483:THR:HG21	1:B:1502:GLN:HA	1.99	0.44
1:A:409:LEU:C	1:A:410:LEU:HD23	2.43	0.44
1:A:438:MET:HE3	1:A:506:GLN:OE1	2.17	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:377:HIS:HE2	1:A:457:GLY:CA	2.28	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:LEU:HD22	1:B:1509:LEU:HD21	1.99	0.44
1:A:313:ASP:OD1	1:A:313:ASP:N	2.50	0.44
1:A:323:GLU:HA	1:A:324:PRO:HD3	1.77	0.44
1:A:396:MET:HE2	1:A:396:MET:HB3	1.73	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:A:421:MET:HE2	1:A:421:MET:HB3	1.53	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: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:B:1397:GLU:C	1:B:1399:PRO:HD3	2.43	0.43
1:A:394:ARG:NH2	1:A:404:PHE:O	2.50	0.43
1:A:431:THR:OG1	1:A:517:MET:HE1	2.19	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:358:ILE:HG21	1:A:543:MET:HE2	2.01	0.43
1:A:396:MET:CE	1:A:436:ARG:HA	2.48	0.43
1:A:458:VAL:O	1:A:472:LYS:NZ	2.50	0.43
1:B:1354:LEU:HD23	1:B:1357:MET:CE	2.48	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: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:B:1391:LEU:HD13	1:B:1404:PHE:CD2	2.54	0.42
1:B:1467:LYS:HA	1:B:1467:LYS:HD2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1388:MET:HG2	1:B:1428:LEU:HD21	2.02	0.41
1:B:1422:VAL:HG13	1:B:1423:GLU:N	2.34	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:1431:THR:OG1	1:B:1517:MET:HE1	2.20	0.41
1:B:1373:HIS:ND1	1:B:1537:TYR:OH	2.54	0.41
1:A:308:LEU:HA	1:A:481:LYS:CD	2.51	0.41
1:A:319:LEU:HD23	1:A:319:LEU:HA	1.95	0.41
1:A:343:MET:O	1:A:346:LEU:HB2	2.21	0.41
1:A:363:ARG:HE	1:A:363:ARG:HB3	1.40	0.41
1:A:343:MET:HE1	2:A:600:IOK:C30	2.49	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
2:A:600:IOK:H81	2:A:600:IOK:C23	2.52	0.40
1:B:1370:LEU:HB3	1:B:1371:THR:H	1.62	0.40
1:B:1460:THR:HG22	1:B:1460:THR:O	2.21	0.40
1:A:413:ASN:OD1	1:A:413:ASN:N	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%)	2	2
1	B	222/254 (87%)	191 (86%)	24 (11%)	7 (3%)	3	3
All	All	443/508 (87%)	383 (86%)	45 (10%)	15 (3%)	3	2

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
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%)	159 (79%)	43 (21%)	1	1
1	B	203/229 (89%)	161 (79%)	42 (21%)	1	1
All	All	405/458 (88%)	320 (79%)	85 (21%)	1	1

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	309	SER
1	A	311	THR
1	A	313	ASP
1	A	315	MET
1	A	321	ASP
1	A	326	ILE
1	A	342	MET
1	A	345	LEU
1	A	349	LEU
1	A	352	ARG
1	A	357	MET
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	431	THR
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	458	VAL
1	A	467	LYS
1	A	468	SER
1	A	469	LEU
1	A	481	LYS
1	A	486	LEU
1	A	487	ILE
1	A	497	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	506	GLN
1	A	512	SER
1	A	514	ILE
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	1315	MET
1	B	1321	ASP
1	B	1326	ILE
1	B	1341	SER
1	B	1342	MET
1	B	1345	LEU
1	B	1349	LEU
1	B	1352	ARG
1	B	1363	ARG
1	B	1368	VAL
1	B	1412	ARG
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	1443	GLU
1	B	1458	VAL
1	B	1462	LEU
1	B	1466	LEU
1	B	1467	LYS
1	B	1468	SER
1	B	1469	LEU
1	B	1475	ILE
1	B	1477	ARG
1	B	1481	LYS
1	B	1486	LEU
1	B	1487	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1492	LYS
1	B	1497	LEU
1	B	1504	LEU
1	B	1506	GLN
1	B	1520	LYS
1	B	1536	LEU
1	B	1542	GLU
1	B	1543	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	ASN
1	A	441	GLN
1	A	476	HIS
1	A	499	GLN
1	A	500	GLN
1	A	524	HIS
1	B	1359	ASN
1	B	1375	GLN
1	B	1441	GLN
1	B	1476	HIS
1	B	1502	GLN
1	B	1519	ASN
1	B	1524	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	-	33,33,33	1.34	3 (9%)	43,45,45	1.27	6 (13%)
2	IOK	B	1600	-	33,33,33	1.33	3 (9%)	43,45,45	1.26	3 (6%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1600	IOK	C17-C16	4.70	1.42	1.38
2	A	600	IOK	C17-C16	4.51	1.42	1.38
2	B	1600	IOK	C24-C16	-2.79	1.39	1.44
2	A	600	IOK	C24-C16	-2.79	1.39	1.44
2	A	600	IOK	C24-C19	-2.42	1.38	1.41
2	B	1600	IOK	C24-C19	-2.35	1.38	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	IOK	C30-C25-C17	-3.71	116.35	120.76
2	B	1600	IOK	C30-C25-C17	-3.47	116.64	120.76
2	A	600	IOK	C26-C25-C17	3.45	124.87	120.76
2	B	1600	IOK	C26-C25-C17	3.18	124.55	120.76
2	A	600	IOK	C8-C9-C10	-2.27	110.47	114.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	IOK	C15-C13-N12	2.22	120.11	116.31
2	A	600	IOK	C19-C24-C16	2.21	108.85	106.84
2	B	1600	IOK	C19-C24-C16	2.10	108.75	106.84
2	A	600	IOK	C16-C17-N18	-2.05	108.14	109.61

There are no chirality outliers.

All (8) torsion outliers are listed below:

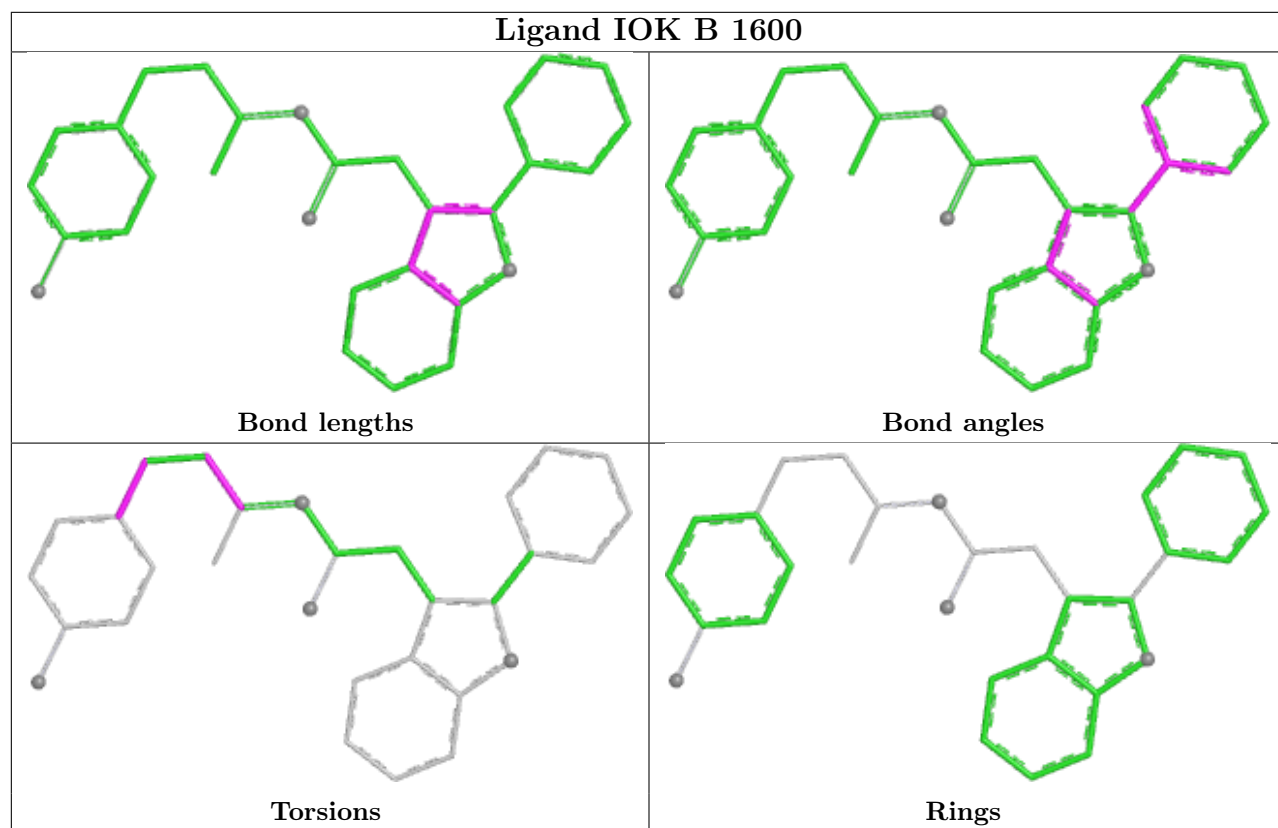
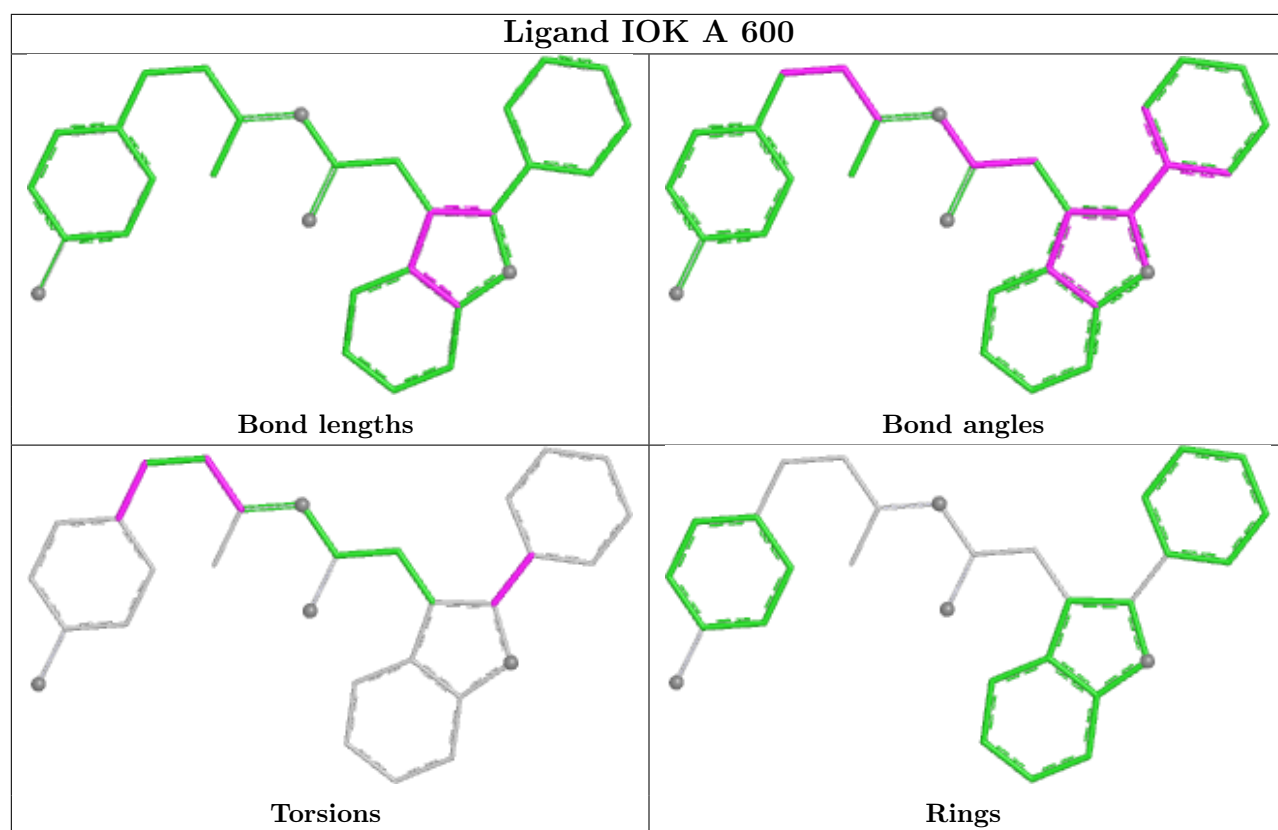
Mol	Chain	Res	Type	Atoms
2	A	600	IOK	C11-C10-C9-C8
2	B	1600	IOK	C11-C10-C9-C8
2	B	1600	IOK	N12-C10-C9-C8
2	A	600	IOK	N12-C10-C9-C8
2	B	1600	IOK	C7-C1-C8-C9
2	B	1600	IOK	C2-C1-C8-C9
2	A	600	IOK	N18-C17-C25-C30
2	A	600	IOK	C7-C1-C8-C9

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	IOK	8	0
2	B	1600	IOK	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/254 (89%)	-0.77	2 (0%) 81 78	13, 41, 83, 104	0
1	B	228/254 (89%)	-0.82	2 (0%) 81 78	14, 41, 83, 104	0
All	All	455/508 (89%)	-0.79	4 (0%) 81 78	13, 41, 84, 104	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	ALA	3.2
1	B	1340	ALA	3.1
1	A	464	SER	2.1
1	B	1457	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

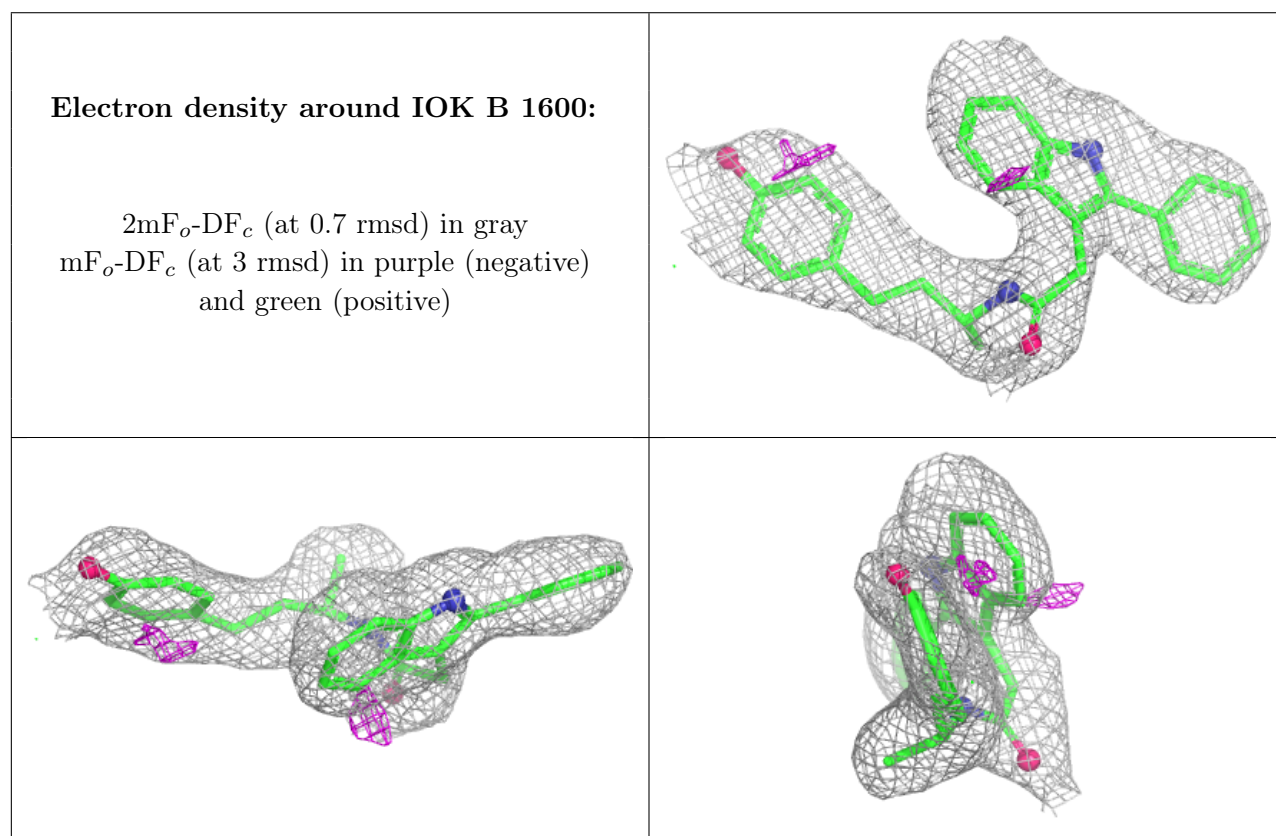
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IOK	B	1600	30/30	0.97	0.06	16,27,41,46	0

Continued on next page...

Continued from previous page...

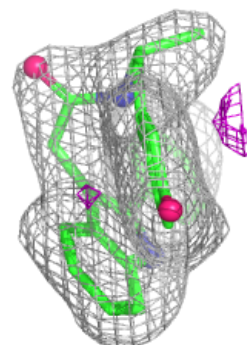
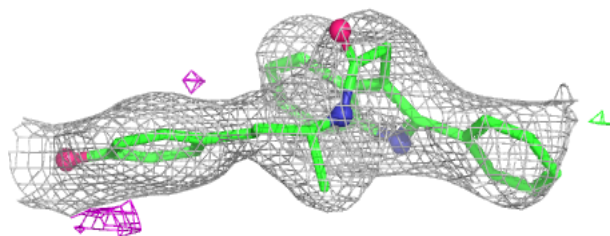
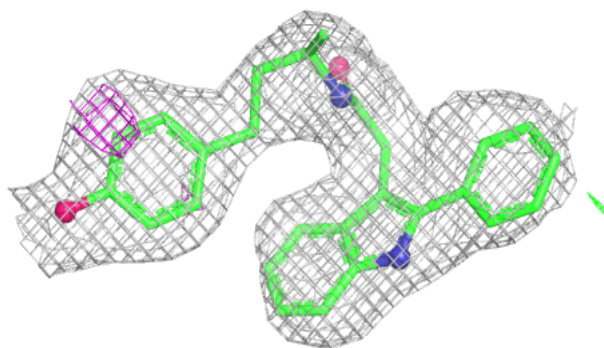
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IOK	A	600	30/30	0.98	0.05	9,33,52,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around IOK A 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.