



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:49 AM UTC

PDB ID : 1X7E / pdb_00001x7e
Title : CRYSTAL STRUCTURE OF ESTROGEN RECEPTOR ALPHA COM-
PLEXED WITH WAY-244
Authors : Manas, E.S.; Unwalla, R.J.; Xu, Z.B.; Malamas, M.S.; Miller, C.P.; Harris,
H.A.; Hsiao, C.; Akopian, T.; Hum, W.T.; Malakian, K.; Wolfrom, S.; Bapat,
A.; Bhat, R.A.; Stahl, M.L.; Somers, W.S.; Alvarez, J.C.
Deposited on : 2004-08-13
Resolution : 2.80 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)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

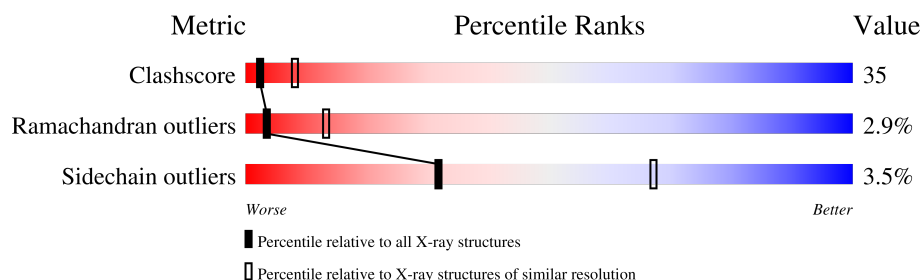
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	245	
1	B	245	
2	C	13	
2	D	13	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4122 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.

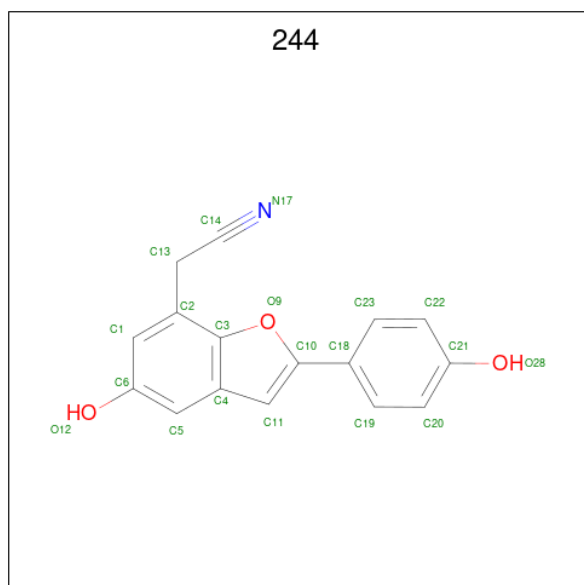
- Molecule 1 is a protein called Estrogen receptor 1 (alpha).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1910	1226	325	340	19			
1	B	238	Total	C	N	O	S	0	0	0
			1910	1226	325	340	19			

- Molecule 2 is a protein called steroid receptor coactivator-3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	0	0
			95	60	20	15			
2	D	11	Total	C	N	O	0	0	0
			95	60	20	15			

- Molecule 3 is [5-HYDROXY-2-(4-HYDROXYPHENYL)-1-BENZOFURAN-7-YL]ACETO NITRILE (CCD ID: 244) (formula: C₁₆H₁₁NO₃).

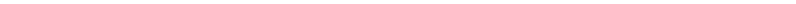


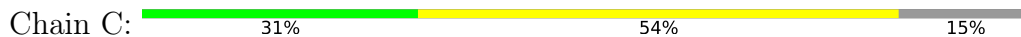
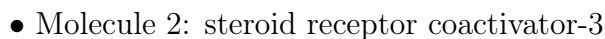
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	16	1	3		
3	B	1	Total	C	N	O	0	0
			20	16	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	34	Total	O	0	0
			34	34		
4	C	2	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			1	1		

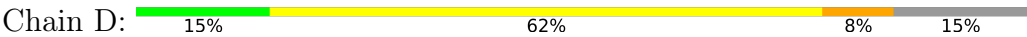
Note EDS was not executed.

- Chain A:  40% 50% 7% ..





● Molecule 2: steroid receptor coactivator-3



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.14Å 79.89Å 59.83Å 90.00° 116.19° 90.00°	Depositor
Resolution (Å)	14.91 – 2.80	Depositor
% Data completeness (in resolution range)	50.0 (14.91-2.80)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4122	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
244

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	0.51	0/1946	0.99	6/2629 (0.2%)
1	B	0.53	2/1946 (0.1%)	1.03	11/2629 (0.4%)
2	C	0.41	0/96	0.88	0/127
2	D	0.44	0/96	0.89	0/127
All	All	0.52	2/4084 (0.0%)	1.01	17/5512 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	422	VAL	C-N	6.00	1.41	1.33
1	B	423	GLU	C-N	-5.53	1.26	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	GLU	N-CA-CB	-9.98	95.07	109.94
1	B	423	GLU	CB-CG-CD	6.87	124.27	112.60
1	B	423	GLU	CG-CD-OE2	-6.84	102.68	118.40
1	B	423	GLU	CB-CA-C	6.56	121.31	110.81
1	B	484	ASP	N-CA-C	-6.23	104.57	111.36
1	B	423	GLU	CG-CD-OE1	6.21	132.69	118.40
1	A	548	ARG	N-CA-C	-6.07	105.58	114.39
1	A	484	ASP	N-CA-C	-5.95	104.71	111.14
1	B	534	VAL	N-CA-C	5.92	113.74	107.76
1	A	397	GLU	N-CA-C	5.62	118.93	112.57
1	B	427	MET	CG-SD-CE	5.40	112.78	100.90
1	A	515	ARG	N-CA-C	-5.40	105.31	111.14
1	B	515	ARG	N-CA-C	-5.21	105.52	111.14
1	B	329	SER	N-CA-C	-5.18	104.04	110.41
1	B	323	GLU	N-CA-C	5.17	115.55	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	ILE	N-CA-C	5.09	117.42	111.05
1	A	423	GLU	CB-CA-C	5.08	118.94	110.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1910	0	1960	153	3
1	B	1910	0	1960	131	2
2	C	95	0	100	10	0
2	D	95	0	100	16	0
3	A	20	0	11	1	0
3	B	20	0	11	0	0
4	A	35	0	0	7	0
4	B	34	0	0	7	1
4	C	2	0	0	0	0
4	D	1	0	0	0	0
All	All	4122	0	4142	289	3

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 35.

All (289) 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:516:HIS:NE2	1:A:520:LYS:HE3	1.61	1.14
1:A:516:HIS:CE1	1:A:520:LYS:HE3	1.96	1.00
1:A:497:LEU:HD11	1:B:497:LEU:HD11	1.41	0.99
1:B:376:VAL:O	1:B:380:GLU:HG3	1.68	0.93
1:B:340:ALA:HA	1:B:533:VAL:HG13	1.50	0.93
1:A:376:VAL:O	1:A:380:GLU:HG3	1.70	0.90
1:B:334:THR:O	1:B:335:ARG:HG3	1.72	0.90
1:B:381:CYS:HB3	4:B:25:HOH:O	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:TYR:CD1	1:A:472:LYS:NZ	2.40	0.89
1:A:498:GLN:O	1:A:502:GLN:HB2	1.77	0.85
1:A:531:LYS:HB2	1:A:533:VAL:HG23	1.62	0.82
1:B:498:GLN:O	1:B:502:GLN:HB2	1.78	0.81
1:B:374:ASP:OD2	1:B:471:GLU:HG2	1.79	0.81
1:A:383:TRP:HZ2	1:A:522:MET:HE1	1.45	0.80
1:A:374:ASP:OD2	1:A:471:GLU:HG2	1.80	0.80
1:B:473:ASP:O	1:B:477:ARG:HG3	1.83	0.78
1:A:473:ASP:O	1:A:477:ARG:HG3	1.82	0.78
1:A:490:MET:O	1:A:495:LEU:HD13	1.86	0.76
1:B:331:TYR:O	1:B:332:ASP:HB2	1.85	0.76
1:A:469:LEU:N	4:A:53:HOH:O	2.19	0.76
1:A:335:ARG:O	1:A:337:PHE:N	2.18	0.75
1:A:516:HIS:NE2	1:A:520:LYS:CE	2.45	0.75
1:A:401:LYS:HD3	1:A:411:ASP:HB3	1.69	0.75
1:A:383:TRP:CZ2	1:A:522:MET:HE1	2.22	0.75
1:A:343:MET:HG3	1:A:528:MET:HE2	1.69	0.74
1:A:459:TYR:CE1	1:A:472:LYS:NZ	2.51	0.73
1:B:340:ALA:HA	1:B:533:VAL:CG1	2.17	0.73
1:B:401:LYS:HD3	1:B:411:ASP:HB3	1.71	0.73
1:A:335:ARG:HG3	1:A:336:PRO:HD2	1.70	0.73
1:A:420:GLY:C	1:A:423:GLU:OE1	2.31	0.73
1:B:343:MET:HG3	1:B:528:MET:HE2	1.71	0.73
1:A:520:LYS:HD3	4:A:71:HOH:O	1.89	0.72
1:B:418:VAL:HG12	1:B:421:MET:HB2	1.71	0.72
1:A:332:ASP:N	1:A:333:PRO:HD3	2.05	0.72
2:D:695:GLN:O	2:D:697:SER:N	2.23	0.71
1:A:332:ASP:H	1:A:333:PRO:HD3	1.56	0.69
1:A:459:TYR:HD1	1:A:472:LYS:NZ	1.91	0.68
1:B:383:TRP:HZ2	1:B:522:MET:HE1	1.59	0.68
1:B:368:VAL:HA	1:B:375:GLN:NE2	2.08	0.68
1:A:539:LEU:HD13	2:C:689:ILE:HG22	1.77	0.67
1:B:332:ASP:C	1:B:334:THR:H	2.02	0.67
1:B:383:TRP:NE1	1:B:543:MET:HB3	2.10	0.66
1:B:539:LEU:HD13	2:D:689:ILE:HG22	1.76	0.66
1:B:531:LYS:O	1:B:532:ASN:HB2	1.96	0.65
1:A:424:ILE:HA	1:A:427:MET:HE3	1.78	0.65
1:A:525:LEU:HD23	1:A:544:LEU:HD13	1.79	0.64
1:B:525:LEU:HD23	1:B:544:LEU:HD13	1.78	0.64
1:A:490:MET:HB3	1:A:495:LEU:HD22	1.78	0.64
1:A:427:MET:HE1	1:A:520:LYS:HD2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:THR:HG23	1:B:499:GLN:OE1	1.99	0.62
1:B:403:LEU:HD11	1:B:406:PRO:HA	1.82	0.61
1:B:422:VAL:HG13	1:B:423:GLU:N	2.14	0.61
2:D:688:LYS:HE2	2:D:688:LYS:N	2.16	0.61
1:A:331:TYR:O	1:A:331:TYR:HD1	1.83	0.61
1:A:459:TYR:CD2	1:B:513:HIS:CE1	2.89	0.61
1:A:542:GLU:OE1	2:C:689:ILE:HB	2.00	0.61
1:B:383:TRP:CZ2	1:B:522:MET:HE1	2.36	0.61
1:B:454:LEU:HB2	1:B:479:LEU:HD21	1.82	0.61
1:B:418:VAL:O	1:B:421:MET:HB3	2.01	0.60
1:B:458:VAL:HG13	1:B:459:TYR:CD1	2.36	0.60
1:B:332:ASP:O	1:B:334:THR:N	2.34	0.60
1:A:454:LEU:HB2	1:A:479:LEU:HD21	1.84	0.59
1:B:424:ILE:HA	1:B:427:MET:HE3	1.84	0.59
1:B:350:ALA:O	1:B:354:LEU:HG	2.02	0.59
1:B:418:VAL:HG11	1:B:421:MET:HE2	1.84	0.59
1:A:342:MET:HE2	1:A:410:LEU:HD13	1.85	0.58
1:A:369:ASP:HB2	1:A:474:HIS:CE1	2.38	0.58
1:B:458:VAL:HG22	1:B:472:LYS:HE3	1.85	0.58
1:B:384:LEU:HD22	1:B:388:MET:SD	2.42	0.58
1:A:306:LEU:HD21	4:A:42:HOH:O	2.03	0.58
1:B:535:PRO:HB2	1:B:537:TYR:CE2	2.39	0.58
1:B:522:MET:HE2	1:B:544:LEU:HD12	1.85	0.58
1:A:497:LEU:HD11	1:B:497:LEU:CD1	2.27	0.58
2:C:688:LYS:N	2:C:688:LYS:HE2	2.18	0.58
2:D:688:LYS:HE2	2:D:688:LYS:CA	2.34	0.58
1:A:350:ALA:O	1:A:354:LEU:HG	2.04	0.57
1:B:369:ASP:HB2	1:B:474:HIS:HE1	1.69	0.57
1:B:380:GLU:OE2	2:D:687:HIS:NE2	2.38	0.57
1:B:422:VAL:CG1	1:B:423:GLU:N	2.68	0.57
1:B:513:HIS:HB3	4:B:14:HOH:O	2.04	0.57
1:A:331:TYR:O	1:A:331:TYR:CD1	2.57	0.57
1:A:427:MET:HE1	1:A:520:LYS:CD	2.34	0.57
1:B:403:LEU:HD12	1:B:405:ALA:O	2.05	0.57
1:B:456:SER:HA	1:B:515:ARG:NH2	2.19	0.57
1:A:531:LYS:O	1:A:533:VAL:HG23	2.05	0.56
1:B:383:TRP:CD1	1:B:543:MET:HB3	2.40	0.56
2:C:688:LYS:HE2	2:C:688:LYS:CA	2.35	0.56
1:A:420:GLY:O	1:A:423:GLU:OE1	2.24	0.56
1:A:456:SER:HA	1:A:515:ARG:NH2	2.21	0.56
1:A:530:CYS:C	1:A:531:LYS:HD3	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:688:LYS:HE2	2:D:688:LYS:HA	1.88	0.55
1:B:496:THR:O	1:B:500:GLN:HG3	2.07	0.55
1:B:376:VAL:HG21	2:D:691:HIS:CE1	2.42	0.55
1:B:397:GLU:O	1:B:397:GLU:HG3	2.06	0.55
1:B:398:HIS:N	1:B:399:PRO:HD3	2.22	0.55
1:A:351:ASP:CG	1:A:537:TYR:HB3	2.32	0.55
1:A:498:GLN:HA	1:A:501:HIS:NE2	2.22	0.55
1:B:311:THR:OG1	1:B:314:GLN:HG3	2.07	0.55
1:A:376:VAL:HG21	2:C:691:HIS:CE1	2.41	0.55
1:A:305:SER:O	1:A:306:LEU:O	2.25	0.55
1:B:366:GLY:O	1:B:474:HIS:HE1	1.89	0.55
1:A:380:GLU:OE2	2:C:687:HIS:NE2	2.39	0.54
1:A:388:MET:HE1	1:A:517:MET:CB	2.36	0.54
1:B:388:MET:HE1	1:B:517:MET:HB2	1.87	0.54
1:B:539:LEU:O	1:B:543:MET:HG2	2.08	0.54
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.89	0.54
1:A:332:ASP:N	1:A:333:PRO:CD	2.70	0.54
1:B:388:MET:HE1	1:B:517:MET:CB	2.38	0.54
1:B:502:GLN:O	1:B:506:GLN:HG3	2.08	0.54
1:B:542:GLU:OE1	2:D:689:ILE:HB	2.07	0.54
1:A:310:LEU:HD12	1:A:310:LEU:O	2.06	0.54
1:A:459:TYR:CE2	1:B:513:HIS:CE1	2.96	0.54
1:A:502:GLN:O	1:A:506:GLN:HG3	2.08	0.54
1:B:396:MET:SD	1:B:435:PHE:HB3	2.48	0.54
1:A:396:MET:SD	1:A:435:PHE:HB3	2.47	0.54
1:A:504:LEU:O	1:A:508:LEU:HG	2.08	0.54
1:A:497:LEU:CD1	1:B:497:LEU:HD11	2.26	0.53
1:A:522:MET:HE2	1:A:544:LEU:HD12	1.89	0.53
1:B:332:ASP:C	1:B:334:THR:N	2.66	0.53
1:A:371:THR:O	1:A:375:GLN:HG3	2.09	0.53
1:B:335:ARG:NH2	1:B:409:LEU:O	2.41	0.53
2:C:688:LYS:HE2	2:C:688:LYS:HA	1.88	0.53
1:A:305:SER:O	1:A:306:LEU:C	2.52	0.53
1:B:368:VAL:HA	1:B:375:GLN:HE22	1.73	0.53
1:A:330:GLU:O	1:A:333:PRO:HD3	2.08	0.53
1:A:403:LEU:HD12	1:A:405:ALA:O	2.08	0.53
1:A:531:LYS:HB2	1:A:533:VAL:CG2	2.37	0.53
1:B:368:VAL:HG13	4:B:8:HOH:O	2.08	0.52
1:A:530:CYS:HB2	1:A:531:LYS:HE3	1.90	0.52
1:B:342:MET:HE2	1:B:410:LEU:HD13	1.91	0.52
1:A:527:SER:O	1:A:531:LYS:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:LEU:HD13	2:D:689:ILE:CG2	2.38	0.52
1:B:503:ARG:HA	1:B:506:GLN:OE1	2.09	0.52
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.91	0.51
1:B:338:SER:H	1:B:341:SER:HB3	1.75	0.51
1:A:538:ASP:O	1:A:542:GLU:HG3	2.11	0.51
1:A:403:LEU:HD13	1:A:409:LEU:HD13	1.91	0.51
1:B:527:SER:O	1:B:531:LYS:HG2	2.10	0.51
1:A:324:PRO:HG3	1:A:360:TRP:HB2	1.92	0.51
1:A:503:ARG:HA	1:A:506:GLN:OE1	2.10	0.51
1:B:383:TRP:CD1	1:B:543:MET:HE3	2.46	0.51
1:A:545:ASP:O	1:A:549:LEU:HD13	2.11	0.51
1:B:331:TYR:O	1:B:333:PRO:HD2	2.10	0.51
1:B:498:GLN:HA	1:B:501:HIS:NE2	2.25	0.51
1:A:388:MET:HE1	1:A:517:MET:HB2	1.92	0.51
1:A:458:VAL:HG13	1:A:459:TYR:CD1	2.46	0.50
1:A:539:LEU:HD13	2:C:689:ILE:CG2	2.40	0.50
1:B:331:TYR:C	1:B:333:PRO:HD2	2.36	0.50
1:B:418:VAL:CG1	1:B:421:MET:HB2	2.41	0.50
1:A:398:HIS:HB3	1:A:401:LYS:HB2	1.94	0.50
1:B:504:LEU:O	1:B:508:LEU:HG	2.12	0.50
1:A:310:LEU:HD11	1:A:315:MET:HE2	1.94	0.50
1:A:368:VAL:C	1:A:370:LEU:N	2.68	0.50
1:A:401:LYS:CD	1:A:411:ASP:HB3	2.41	0.49
1:A:423:GLU:CD	1:A:423:GLU:H	2.19	0.49
1:A:368:VAL:HA	1:A:375:GLN:NE2	2.28	0.49
1:A:330:GLU:OE1	1:A:345:LEU:HD23	2.12	0.49
1:A:513:HIS:HB3	4:A:51:HOH:O	2.11	0.49
1:A:384:LEU:HD22	1:A:388:MET:SD	2.53	0.49
1:B:308:LEU:HD21	1:B:478:VAL:HA	1.94	0.49
1:A:331:TYR:CD1	1:A:331:TYR:C	2.90	0.49
1:B:397:GLU:O	1:B:397:GLU:CG	2.61	0.48
2:D:696:ASP:O	2:D:697:SER:C	2.56	0.48
1:A:377:HIS:NE2	1:A:460:THR:HB	2.29	0.48
1:A:421:MET:HE1	3:A:201:244:C1	2.44	0.48
1:B:308:LEU:HA	1:B:481:LYS:HG3	1.95	0.48
1:B:305:SER:O	1:B:306:LEU:O	2.31	0.48
1:B:367:PHE:C	1:B:369:ASP:H	2.22	0.48
1:B:403:LEU:HD13	1:B:409:LEU:HD13	1.95	0.48
1:B:538:ASP:O	1:B:542:GLU:HG3	2.14	0.48
1:A:458:VAL:HG23	1:A:475:ILE:HD12	1.94	0.48
1:A:539:LEU:O	1:A:543:MET:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:THR:OG1	1:A:314:GLN:HG3	2.14	0.48
1:A:306:LEU:C	1:A:308:LEU:H	2.22	0.47
1:A:371:THR:HG23	1:A:471:GLU:OE1	2.14	0.47
1:A:451:ILE:HG13	1:A:482:ILE:HG21	1.96	0.47
1:B:362:LYS:HE2	2:D:694:LEU:O	2.15	0.47
1:A:339:GLU:HG3	1:A:418:VAL:HG13	1.96	0.47
1:B:456:SER:C	4:B:25:HOH:O	2.58	0.47
1:B:369:ASP:HB2	1:B:474:HIS:CE1	2.48	0.47
1:B:456:SER:HB3	4:B:25:HOH:O	2.15	0.47
1:B:498:GLN:HG2	1:B:502:GLN:OE1	2.15	0.47
1:A:323:GLU:HA	1:A:324:PRO:HD3	1.78	0.46
1:B:451:ILE:HG13	1:B:482:ILE:HG21	1.96	0.46
1:B:338:SER:N	1:B:341:SER:HB3	2.30	0.46
1:A:528:MET:HB3	1:A:534:VAL:HG23	1.98	0.46
1:A:329:SER:OG	1:A:330:GLU:N	2.48	0.46
1:A:366:GLY:O	1:A:474:HIS:HE1	1.99	0.46
1:A:498:GLN:HG2	1:A:502:GLN:OE1	2.15	0.46
1:A:335:ARG:O	1:A:336:PRO:C	2.57	0.46
1:A:343:MET:HE2	1:A:528:MET:HG3	1.98	0.46
1:B:388:MET:CE	1:B:517:MET:HB2	2.46	0.46
1:B:327:LEU:HD11	1:B:356:HIS:CD2	2.51	0.46
1:B:448:LEU:HD21	1:B:507:LEU:HB3	1.97	0.46
2:D:695:GLN:C	2:D:697:SER:N	2.73	0.46
1:B:458:VAL:HG13	1:B:459:TYR:HD1	1.79	0.46
1:A:395:SER:HB3	4:A:30:HOH:O	2.14	0.46
1:B:401:LYS:CD	1:B:411:ASP:HB3	2.43	0.46
1:A:328:TYR:CE2	1:A:406:PRO:HB2	2.51	0.45
1:B:367:PHE:C	1:B:369:ASP:N	2.72	0.45
1:A:333:PRO:O	1:A:334:THR:HB	2.16	0.45
1:A:487:ILE:HG13	1:B:501:HIS:CG	2.51	0.45
1:A:403:LEU:HA	1:A:409:LEU:HD12	1.97	0.45
1:A:448:LEU:HD21	1:A:507:LEU:HB3	1.99	0.45
1:B:418:VAL:O	1:B:421:MET:CB	2.64	0.45
1:A:362:LYS:HE2	2:C:694:LEU:O	2.16	0.44
1:B:312:ALA:HB1	1:B:488:HIS:ND1	2.32	0.44
1:B:366:GLY:O	1:B:369:ASP:HB2	2.17	0.44
1:B:380:GLU:O	1:B:547:HIS:NE2	2.50	0.44
1:A:397:GLU:HB3	4:A:2:HOH:O	2.17	0.44
1:A:474:HIS:CD2	4:A:67:HOH:O	2.70	0.44
1:A:527:SER:O	1:A:531:LYS:HE3	2.17	0.44
1:B:471:GLU:OE2	1:B:471:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:THR:HG21	1:A:534:VAL:HG13	1.98	0.44
1:A:522:MET:HE2	1:A:544:LEU:HA	1.99	0.44
1:B:307:ALA:CB	1:B:365:PRO:HB3	2.46	0.44
1:A:400:VAL:HG12	1:A:400:VAL:O	2.18	0.44
1:A:503:ARG:HG3	1:A:503:ARG:HH11	1.82	0.44
1:B:377:HIS:NE2	1:B:460:THR:HB	2.33	0.44
1:B:403:LEU:HA	1:B:409:LEU:HD12	1.99	0.44
1:A:530:CYS:O	1:A:531:LYS:HD3	2.18	0.44
1:B:343:MET:HE2	1:B:528:MET:HG3	1.99	0.43
1:B:402:LEU:HG	1:B:429:LEU:HD21	2.00	0.43
1:A:310:LEU:CD1	1:A:315:MET:HB2	2.48	0.43
1:B:354:LEU:HD13	1:B:543:MET:HG3	1.99	0.43
1:B:358:ILE:HG21	2:D:693:LEU:HB3	2.00	0.43
1:B:360:TRP:CH2	1:B:449:LYS:HG2	2.53	0.43
1:A:383:TRP:CE2	1:A:543:MET:HB3	2.54	0.43
1:A:354:LEU:HD13	1:A:543:MET:HG3	2.01	0.43
1:A:501:HIS:CG	1:B:487:ILE:HG13	2.54	0.43
1:A:531:LYS:CB	1:A:533:VAL:HG23	2.42	0.43
1:B:383:TRP:CE2	1:B:543:MET:HB3	2.54	0.43
2:D:695:GLN:O	2:D:696:ASP:C	2.62	0.43
2:D:695:GLN:C	2:D:697:SER:H	2.27	0.43
1:A:322:ALA:HB1	1:A:363:ARG:HB2	2.01	0.43
1:A:536:LEU:HG	1:A:541:LEU:HD21	2.00	0.43
1:A:358:ILE:HG21	2:C:693:LEU:HB3	2.01	0.43
1:B:323:GLU:HA	1:B:324:PRO:HD3	1.71	0.43
1:A:367:PHE:O	1:A:370:LEU:HB2	2.19	0.43
1:A:531:LYS:O	1:A:532:ASN:C	2.62	0.43
1:B:398:HIS:N	1:B:399:PRO:CD	2.82	0.43
1:A:433:SER:O	1:A:437:MET:HB2	2.19	0.42
1:A:380:GLU:O	1:A:547:HIS:NE2	2.52	0.42
1:A:493:ALA:HB3	1:A:495:LEU:CD1	2.49	0.42
1:B:307:ALA:HB2	1:B:365:PRO:HB3	2.01	0.42
1:B:400:VAL:HG12	1:B:400:VAL:O	2.19	0.42
1:A:388:MET:CE	1:A:517:MET:HB2	2.49	0.42
1:A:533:VAL:O	1:A:533:VAL:HG12	2.19	0.42
1:A:383:TRP:NE1	1:A:543:MET:HB3	2.34	0.42
1:B:322:ALA:HB1	1:B:363:ARG:HB2	2.02	0.42
1:B:493:ALA:HB3	1:B:495:LEU:HD13	2.02	0.42
1:B:526:TYR:CD1	1:B:526:TYR:C	2.98	0.42
1:B:548:ARG:NH1	4:B:72:HOH:O	2.53	0.42
1:A:368:VAL:C	1:A:370:LEU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ILE:HD11	1:A:511:LEU:HD22	2.01	0.41
1:A:471:GLU:OE2	1:A:471:GLU:HA	2.20	0.41
1:A:526:TYR:CD1	1:A:526:TYR:C	2.98	0.41
1:B:371:THR:O	1:B:375:GLN:HG3	2.20	0.41
1:B:472:LYS:HB3	1:B:472:LYS:HE2	1.87	0.41
1:B:522:MET:HE2	1:B:544:LEU:HA	2.01	0.41
1:A:405:ALA:HB3	1:A:408:LEU:HB3	2.02	0.41
1:A:458:VAL:HG22	1:A:472:LYS:HE3	2.02	0.41
1:A:307:ALA:HB2	1:A:365:PRO:C	2.45	0.41
1:B:397:GLU:O	1:B:398:HIS:ND1	2.53	0.41
1:A:312:ALA:CB	1:A:488:HIS:ND1	2.84	0.41
1:A:333:PRO:C	1:A:335:ARG:H	2.28	0.41
1:A:342:MET:HE2	1:A:410:LEU:CD1	2.51	0.41
1:A:342:MET:HE1	1:A:414:GLN:HB3	2.03	0.41
1:A:360:TRP:CH2	1:A:449:LYS:HG2	2.56	0.41
1:A:368:VAL:O	1:A:370:LEU:N	2.54	0.41
1:A:390:GLY:O	1:A:394:ARG:HG3	2.21	0.41
1:B:397:GLU:HB3	4:B:34:HOH:O	2.20	0.41
1:B:405:ALA:O	1:B:406:PRO:C	2.62	0.41
1:B:433:SER:O	1:B:437:MET:HB2	2.21	0.41
1:B:497:LEU:HD23	1:B:497:LEU:HA	1.97	0.41
1:A:368:VAL:O	1:A:369:ASP:C	2.64	0.41
1:A:427:MET:HB3	1:A:517:MET:SD	2.61	0.41
1:B:378:LEU:HA	1:B:378:LEU:HD23	1.87	0.41
1:A:486:LEU:O	1:A:490:MET:HG3	2.21	0.40
1:B:332:ASP:O	1:B:334:THR:OG1	2.38	0.40
1:B:335:ARG:HE	1:B:414:GLN:HE22	1.68	0.40
1:B:452:ILE:HD11	1:B:511:LEU:HD22	2.02	0.40
1:A:319:LEU:HB3	1:A:446:VAL:HB	2.03	0.40
1:A:395:SER:O	1:A:396:MET:C	2.63	0.40
1:A:475:ILE:O	1:A:479:LEU:HG	2.21	0.40
1:B:312:ALA:CB	1:B:488:HIS:ND1	2.84	0.40
1:A:339:GLU:HA	1:A:418:VAL:HG22	2.04	0.40
1:A:472:LYS:HE2	1:A:472:LYS:HB3	1.88	0.40
2:D:687:HIS:C	2:D:688:LYS:HE2	2.46	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:VAL:CG2	4:B:36:HOH:O[2_646]	1.51	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:VAL:CB	1:B:419:GLU:OE2[2_646]	2.08	0.12
1:A:400:VAL:CG1	1:B:419:GLU:OE2[2_646]	2.17	0.03

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	234/245 (96%)	213 (91%)	14 (6%)	7 (3%)	3	12
1	B	234/245 (96%)	217 (93%)	12 (5%)	5 (2%)	5	20
2	C	9/13 (69%)	8 (89%)	0	1 (11%)	0	1
2	D	9/13 (69%)	8 (89%)	0	1 (11%)	0	1
All	All	486/516 (94%)	446 (92%)	26 (5%)	14 (3%)	3	13

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	333	PRO
1	A	336	PRO
1	A	400	VAL
1	B	306	LEU
1	B	332	ASP
1	B	334	THR
1	B	400	VAL
2	D	696	ASP
1	A	307	ALA
1	A	332	ASP
2	C	696	ASP
1	B	333	PRO
1	A	337	PHE

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	215/222 (97%)	206 (96%)	9 (4%)	26	61
1	B	215/222 (97%)	208 (97%)	7 (3%)	33	69
2	C	11/13 (85%)	11 (100%)	0	100	100
2	D	11/13 (85%)	11 (100%)	0	100	100
All	All	452/470 (96%)	436 (96%)	16 (4%)	32	67

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	ASP
1	A	336	PRO
1	A	368	VAL
1	A	384	LEU
1	A	477	ARG
1	A	486	LEU
1	A	527	SER
1	A	541	LEU
1	A	549	LEU
1	B	334	THR
1	B	384	LEU
1	B	477	ARG
1	B	486	LEU
1	B	527	SER
1	B	536	LEU
1	B	541	LEU

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

Mol	Chain	Res	Type
1	A	359	ASN
1	A	375	GLN
1	A	474	HIS

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Mol	Chain	Res	Type
1	A	519	ASN
1	B	356	HIS
1	B	359	ASN
1	B	375	GLN
1	B	474	HIS
1	B	513	HIS
2	C	691	HIS
2	D	691	HIS

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 oligosaccharides 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	$\# Z > 2$
3	244	B	202	-	22,22,22	3.33	15 (68%)	28,31,31	1.62	5 (17%)
3	244	A	201	-	22,22,22	3.21	14 (63%)	28,31,31	1.53	5 (17%)

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
3	244	B	202	-	-	0/6/7/7	0/3/3/3
3	244	A	201	-	-	0/6/7/7	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	244	C4-C3	6.17	1.47	1.40
3	A	201	244	C4-C3	5.94	1.47	1.40
3	B	202	244	C19-C18	5.35	1.47	1.39
3	B	202	244	C23-C18	5.08	1.47	1.39
3	A	201	244	C23-C18	5.03	1.47	1.39
3	A	201	244	C19-C18	4.73	1.46	1.39
3	B	202	244	C5-C6	4.69	1.46	1.39
3	A	201	244	C5-C6	4.38	1.45	1.39
3	A	201	244	C11-C10	4.23	1.43	1.35
3	B	202	244	C11-C10	4.20	1.43	1.35
3	A	201	244	C1-C6	4.11	1.45	1.39
3	B	202	244	C1-C6	4.10	1.45	1.39
3	B	202	244	C22-C21	4.00	1.46	1.39
3	A	201	244	C1-C2	3.77	1.45	1.39
3	A	201	244	C22-C21	3.66	1.45	1.39
3	B	202	244	C23-C22	3.57	1.44	1.38
3	B	202	244	C1-C2	3.56	1.45	1.39
3	A	201	244	C20-C19	3.40	1.44	1.38
3	B	202	244	C20-C19	3.35	1.44	1.38
3	A	201	244	C23-C22	3.32	1.44	1.38
3	A	201	244	O9-C10	-2.99	1.35	1.39
3	B	202	244	C5-C4	2.84	1.45	1.40
3	B	202	244	C20-C21	2.74	1.44	1.39
3	A	201	244	C20-C21	2.72	1.44	1.39
3	B	202	244	C3-C2	2.65	1.45	1.40
3	A	201	244	C5-C4	2.56	1.45	1.40
3	A	201	244	C3-C2	2.31	1.44	1.40
3	B	202	244	O9-C10	-2.30	1.36	1.39
3	B	202	244	C13-C14	2.01	1.49	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	244	C4-C11-C10	-3.89	102.97	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	244	C3-C4-C11	3.72	107.91	105.31
3	A	201	244	C4-C11-C10	-3.51	103.40	107.41
3	A	201	244	C3-C4-C11	3.21	107.55	105.31
3	B	202	244	O9-C10-C11	3.20	113.65	110.85
3	A	201	244	O9-C10-C11	3.04	113.50	110.85
3	B	202	244	O9-C3-C4	-2.82	108.27	110.46
3	A	201	244	O9-C3-C4	-2.80	108.29	110.46
3	B	202	244	C18-C10-C11	-2.43	126.48	133.04
3	A	201	244	C18-C10-C11	-2.40	126.56	133.04

There are no chirality outliers.

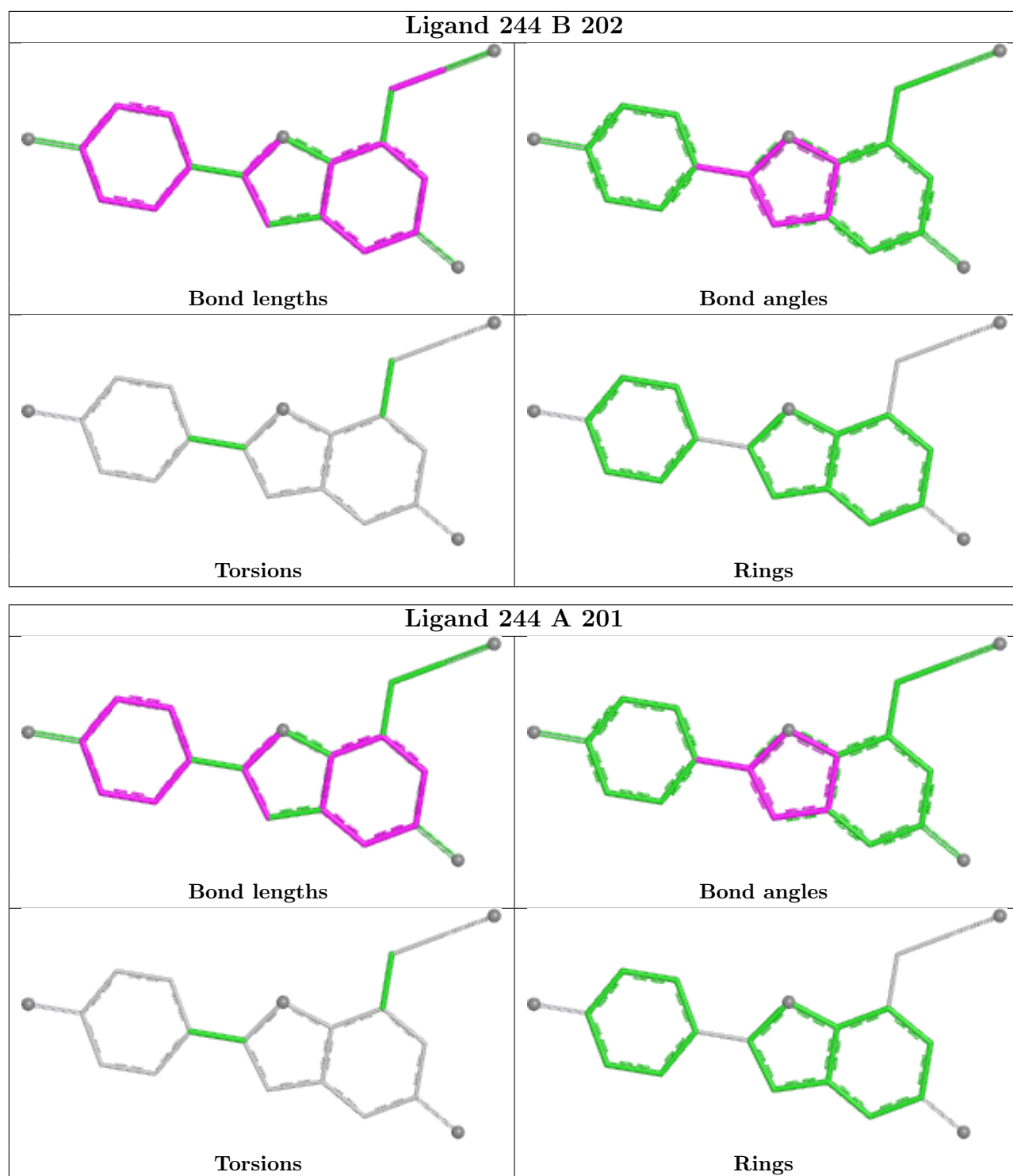
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	244	1	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.