WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:47 pm GMT

PDB ID	:	4DK8
Title	:	Crystal structure of LXR ligand binding domain in complex with partial agonist 5
Authors	:	Piper, D.E.; Kopecky, D.J.; Xu, H.
Deposited on	:	2012-02-03
Resolution	:	2.75 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:

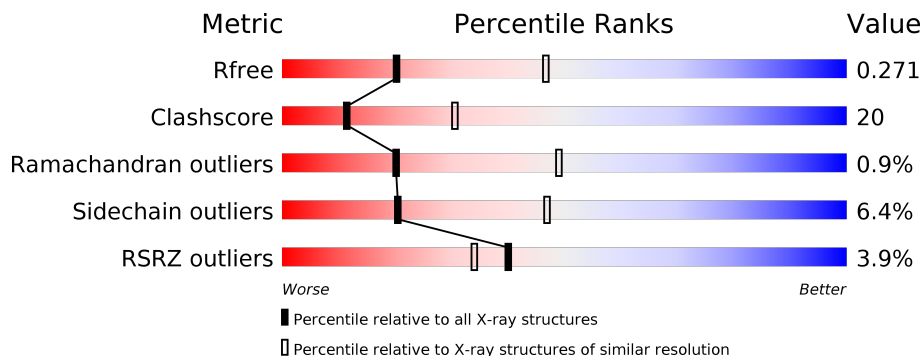|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.75 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	Percentile Ranks	Value
Rfree		0.271
Clashscore		20
Ramachandran outliers		0.9%
Sidechain outliers		6.4%
RSRZ outliers		3.9%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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 <=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	247	4% — 60% / 31% / • 6%
1	C	247	4% — 51% / 36% / 5% / 7%
2	B	12	50% / 50%
2	D	12	58% / 42%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	0KT	A	501	-	-	-	X
5	CA	A	503	-	-	-	X
5	CA	C	502	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 4081 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 Oxysterols receptor LXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total 1905	C 1217	N 336	O 344	S 8	0	0	0
1	C	229	Total 1870	C 1199	N 328	O 336	S 7	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	GLY	-	EXPRESSION TAG	UNP P55055
A	216	SER	-	EXPRESSION TAG	UNP P55055
A	217	HIS	-	EXPRESSION TAG	UNP P55055
A	218	MET	-	EXPRESSION TAG	UNP P55055
C	215	GLY	-	EXPRESSION TAG	UNP P55055
C	216	SER	-	EXPRESSION TAG	UNP P55055
C	217	HIS	-	EXPRESSION TAG	UNP P55055
C	218	MET	-	EXPRESSION TAG	UNP P55055

- Molecule 2 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	12	Total 108	C 68	N 19	O 21	0	0	0
2	D	12	Total 108	C 68	N 19	O 21	0	0	0

- Molecule 3 is N-METHYL-N-(4-{(1S)-2,2,2-TRIFLUORO-1-HYDROXY-1-[1-(2-METHOXYETHYL)-1H-PYRROL-2-YL]ETHYL}PHENYL)BENZENESULFONAMIDE (three-letter code: 0KT) (formula: $C_{22}H_{23}F_3N_2O_4S$).
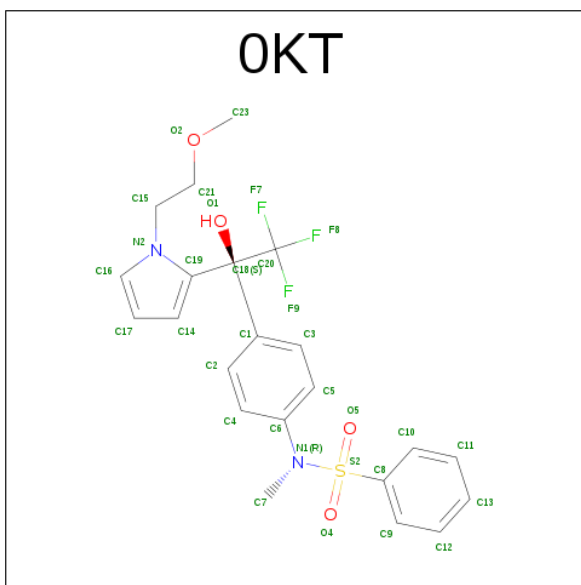
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S		0	0
			32	22	3	2	4	1			
3	C	1	Total	C	F	N	O	S		0	0
			32	22	3	2	4	1			

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
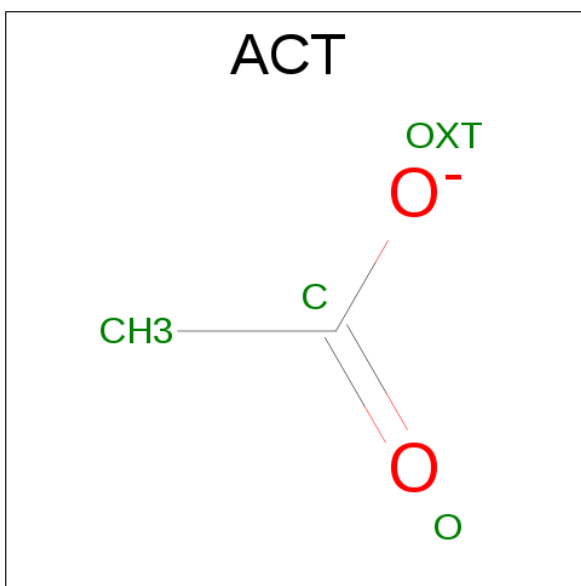
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total 4	Ca 4	0	0
5	C	2	Total 2	Ca 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total 8	O 8	0	0
6	C	7	Total 7	O 7	0	0
6	D	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Oxysterols receptor LXR-beta
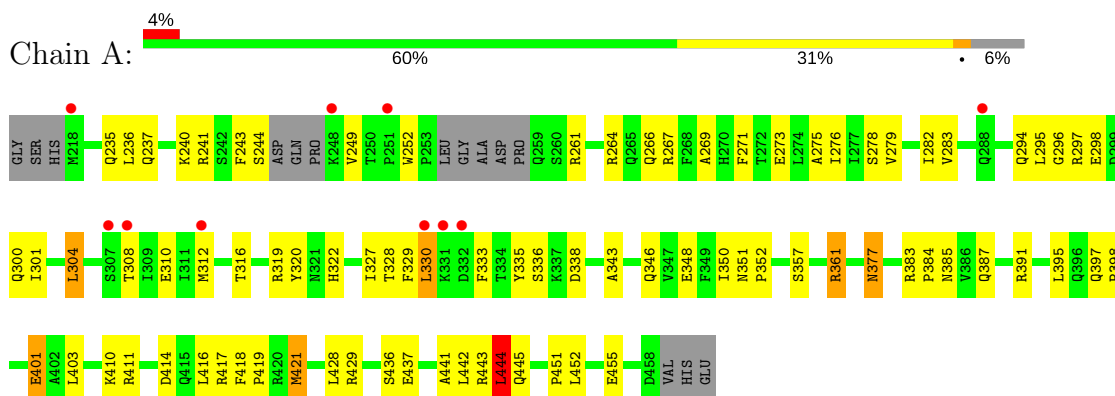
Chain A:

• Molecule 1: Oxysterols receptor LXR-beta
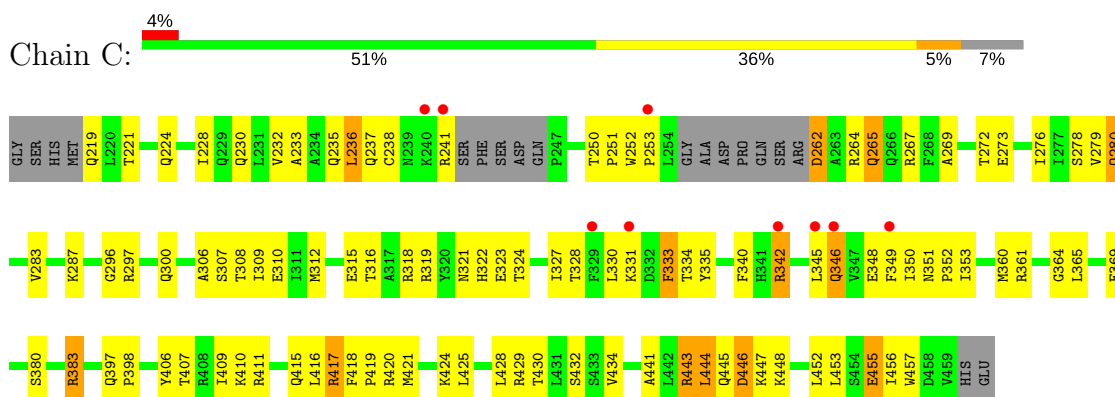
Chain C:

• Molecule 2: Nuclear receptor coactivator 1

Chain B:

• Molecule 2: Nuclear receptor coactivator 1

Chain D:

D365 H366 Q367 L368 L369 R370 Y371 L372 D376

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.14Å 88.14Å 198.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.73 – 2.75 29.73 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.73-2.75) 99.5 (29.73-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.76Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.278 0.241 , 0.271	Depositor DCC
R_{free} test set	1076 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	81.6	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.6	EDS
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4081	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 0KT, ACT

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	0.41	0/1940	0.52	0/2618
1	C	0.37	0/1905	0.51	0/2574
2	B	0.41	0/109	0.47	0/144
2	D	0.46	0/109	0.57	0/144
All	All	0.39	0/4063	0.52	0/5480

There are no bond length outliers.

There are no bond angle outliers.

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	1905	0	1934	72	0
1	C	1870	0	1908	85	0
2	B	108	0	105	5	0
2	D	108	0	105	5	0
3	A	32	0	23	3	0
3	C	32	0	23	0	0
4	A	4	0	3	0	0
5	A	4	0	0	0	0
5	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	8	0	0	0	0
6	C	7	0	0	0	0
6	D	1	0	0	0	0
All	All	4081	0	4101	161	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 20.

All (161) 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:C:310:GLU:HG2	1:C:428:LEU:HB3	1.50	0.94
1:A:444:LEU:H	1:A:444:LEU:HD23	1.35	0.92
1:A:237:GLN:HE21	1:A:241:ARG:HH12	1.26	0.82
1:C:235:GLN:HE21	1:C:318:ARG:HH12	1.26	0.81
1:C:328:THR:HG22	1:C:334:THR:HG22	1.64	0.79
1:C:235:GLN:HE21	1:C:318:ARG:NH1	1.81	0.79
1:C:418:PHE:HB3	1:C:419:PRO:HD3	1.66	0.76
2:D:366:HIS:O	2:D:370:ARG:HG3	1.87	0.75
1:C:252:TRP:CH2	1:C:267:ARG:HD3	2.22	0.74
1:A:442:LEU:HD11	3:A:501:0KT:H6	1.69	0.73
1:C:349:PHE:O	1:C:353:ILE:HG12	1.88	0.73
1:A:295:LEU:HA	1:A:391:ARG:HH21	1.53	0.73
1:A:237:GLN:HE21	1:A:241:ARG:NH1	1.88	0.72
1:A:310:GLU:HB3	1:A:428:LEU:HD13	1.73	0.70
1:C:269:ALA:O	1:C:273:GLU:HG3	1.91	0.70
1:A:336:SER:OG	1:A:338:ASP:HB3	1.91	0.70
1:C:446:ASP:O	1:C:447:LYS:HG3	1.93	0.69
1:C:452:LEU:HB3	2:D:368:LEU:HD22	1.73	0.69
1:C:316:THR:HG23	1:C:327:ILE:HG21	1.75	0.67
1:A:403:LEU:HD11	1:A:421:MET:HE1	1.75	0.66
1:A:266:GLN:O	1:A:269:ALA:HB3	1.96	0.65
1:A:295:LEU:HA	1:A:391:ARG:NH2	2.10	0.65
1:C:265:GLN:HE21	1:C:265:GLN:HA	1.61	0.65
1:A:294:GLN:O	1:A:391:ARG:NH2	2.28	0.65
1:A:410:LYS:O	1:A:411:ARG:HG3	1.98	0.63
1:A:418:PHE:HB3	1:A:419:PRO:HD3	1.82	0.62
1:C:410:LYS:CG	1:C:411:ARG:HG3	2.30	0.62
1:C:410:LYS:HG2	1:C:411:ARG:HG3	1.81	0.62
1:C:322:HIS:HD2	1:C:361:ARG:HD2	1.65	0.61
1:C:310:GLU:CD	1:C:383:ARG:HH22	2.04	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLN:O	1:A:304:LEU:HD12	2.00	0.61
1:C:272:THR:O	1:C:276:ILE:HG13	2.01	0.61
1:A:377:ASN:HD21	1:A:383:ARG:HH21	1.50	0.60
1:C:330:LEU:O	1:C:331:LYS:HG3	2.02	0.59
1:C:417:ARG:HH11	1:C:417:ARG:HG2	1.66	0.59
1:C:235:GLN:NE2	1:C:318:ARG:HH12	1.97	0.59
1:A:441:ALA:O	1:A:445:GLN:HG3	2.03	0.59
1:A:444:LEU:H	1:A:444:LEU:CD2	2.03	0.59
1:C:456:ILE:HG22	1:C:457:TRP:CD1	2.37	0.59
1:A:296:GLY:O	1:A:300:GLN:HG3	2.03	0.58
1:C:228:ILE:O	1:C:232:VAL:HG23	2.02	0.58
1:C:406:TYR:O	1:C:410:LYS:HB3	2.04	0.58
1:A:316:THR:CG2	1:A:327:ILE:HD13	2.33	0.58
1:C:380:SER:HB2	1:C:383:ARG:HD3	1.86	0.58
1:A:330:LEU:HB2	1:A:333:PHE:HB2	1.85	0.57
1:A:403:LEU:HD21	1:A:421:MET:HE3	1.86	0.57
2:B:372:LEU:O	2:B:375:LYS:HG2	2.03	0.57
1:A:319:ARG:HD3	1:A:328:THR:O	2.04	0.57
1:A:252:TRP:CZ2	1:A:267:ARG:HD3	2.40	0.57
1:C:235:GLN:HE21	1:C:318:ARG:CZ	2.17	0.57
1:A:279:VAL:O	1:A:283:VAL:HG23	2.04	0.56
1:A:377:ASN:C	1:A:377:ASN:HD22	2.09	0.56
1:A:297:ARG:HD3	1:A:297:ARG:O	2.05	0.56
1:A:252:TRP:CH2	1:A:267:ARG:HD3	2.40	0.56
1:A:320:TYR:CE2	1:A:322:HIS:HA	2.40	0.56
1:A:283:VAL:HG22	1:A:304:LEU:CD2	2.35	0.56
1:C:235:GLN:HE21	1:C:318:ARG:NH2	2.04	0.56
1:A:330:LEU:HD12	1:A:333:PHE:CG	2.41	0.55
1:C:416:LEU:O	1:C:420:ARG:HD3	2.07	0.55
1:C:333:PHE:HD2	1:C:333:PHE:H	1.54	0.54
1:C:296:GLY:O	1:C:300:GLN:HG3	2.07	0.54
1:A:237:GLN:NE2	1:A:241:ARG:HH12	2.01	0.54
1:C:221:THR:OG1	1:C:224:GLN:HG3	2.06	0.54
1:A:444:LEU:N	1:A:444:LEU:HD23	2.13	0.53
1:A:319:ARG:NH1	1:A:329:PHE:CE2	2.76	0.53
1:C:235:GLN:NE2	1:C:318:ARG:HH22	2.06	0.53
1:A:271:PHE:CE1	3:A:501:0KT:H22	2.44	0.53
1:A:335:TYR:N	1:A:335:TYR:CD1	2.77	0.52
1:C:219:GLN:O	1:C:219:GLN:HG2	2.08	0.52
1:C:322:HIS:CD2	1:C:361:ARG:HD2	2.43	0.52
1:A:416:LEU:C	1:A:419:PRO:HD2	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:ALA:O	1:C:445:GLN:HG3	2.11	0.51
1:C:417:ARG:NH1	1:C:417:ARG:HG2	2.25	0.51
1:C:235:GLN:HE21	1:C:318:ARG:HH22	1.57	0.51
1:A:357:SER:O	1:A:361:ARG:HB2	2.11	0.50
2:D:368:LEU:O	2:D:372:LEU:HG	2.11	0.50
1:A:278:SER:O	1:A:282:ILE:HG13	2.12	0.50
1:C:345:LEU:N	1:C:345:LEU:HD12	2.26	0.50
1:C:264:ARG:HG3	1:C:265:GLN:N	2.26	0.50
1:C:453:LEU:HD22	1:C:457:TRP:CZ3	2.47	0.50
1:A:283:VAL:HG22	1:A:304:LEU:HD22	1.94	0.49
1:C:342:ARG:H	1:C:342:ARG:HD3	1.78	0.49
1:A:275:ALA:O	1:A:279:VAL:HG23	2.12	0.49
2:B:368:LEU:O	2:B:371:TYR:HB3	2.13	0.49
1:A:343:ALA:O	3:A:501:0KT:H9	2.13	0.49
2:B:375:LYS:O	2:B:376:ASP:HB2	2.12	0.49
1:A:351:ASN:HB2	1:A:352:PRO:HD3	1.95	0.48
1:A:377:ASN:HD21	1:A:383:ARG:NH2	2.10	0.48
1:A:330:LEU:HD12	1:A:333:PHE:CD2	2.48	0.48
1:C:308:THR:HG22	1:C:312:MET:HE3	1.96	0.48
1:C:360:MET:SD	1:C:424:LYS:HG3	2.54	0.48
1:A:346:GLN:HB2	1:A:348:GLU:OE1	2.14	0.48
1:A:384:PRO:O	1:A:385:ASN:HB2	2.14	0.48
1:A:276:ILE:HG23	1:A:452:LEU:HD23	1.95	0.48
1:C:280:GLN:HE21	1:C:280:GLN:HB2	1.51	0.48
1:C:416:LEU:C	1:C:419:PRO:HD2	2.34	0.48
1:A:297:ARG:O	1:A:301:ILE:HG12	2.15	0.47
1:A:308:THR:O	1:A:312:MET:HG3	2.13	0.47
1:A:397:GLN:N	1:A:398:PRO:HD2	2.30	0.47
1:C:452:LEU:HD22	2:D:368:LEU:HB2	1.97	0.47
1:A:377:ASN:O	1:A:377:ASN:ND2	2.48	0.47
1:A:346:GLN:O	1:A:350:ILE:HG13	2.15	0.46
1:A:451:PRO:O	1:A:455:GLU:HB2	2.15	0.46
1:C:283:VAL:O	1:C:287:LYS:HG3	2.15	0.46
1:C:351:ASN:HB2	1:C:352:PRO:HD3	1.97	0.46
1:A:377:ASN:C	1:A:377:ASN:ND2	2.69	0.46
1:C:310:GLU:OE2	1:C:383:ARG:NH2	2.48	0.46
1:C:444:LEU:C	1:C:446:ASP:H	2.19	0.46
1:A:403:LEU:HD11	1:A:421:MET:CE	2.43	0.46
1:C:321:ASN:HB3	1:C:324:THR:OG1	2.16	0.45
1:A:361:ARG:HA	1:A:361:ARG:HD3	1.78	0.45
1:C:333:PHE:HB3	1:C:335:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ARG:HD3	1:A:417:ARG:HD2	1.99	0.45
1:C:230:GLN:O	1:C:233:ALA:HB3	2.17	0.45
1:C:262:ASP:O	1:C:265:GLN:HB2	2.16	0.45
2:B:375:LYS:O	2:B:376:ASP:CB	2.64	0.45
1:A:377:ASN:ND2	1:A:383:ARG:HH21	2.13	0.44
1:C:236:LEU:C	1:C:236:LEU:HD12	2.38	0.44
1:C:333:PHE:N	1:C:333:PHE:CD2	2.85	0.44
1:C:429:ARG:O	1:C:432:SER:HB3	2.18	0.44
1:C:253:PRO:HG2	1:C:267:ARG:HG2	2.00	0.44
1:C:411:ARG:HE	1:C:411:ARG:HB3	1.47	0.44
1:A:301:ILE:HG23	2:B:369:LEU:HD23	1.99	0.44
1:A:264:ARG:HE	1:A:264:ARG:HB3	1.63	0.44
1:C:418:PHE:HB3	1:C:419:PRO:CD	2.44	0.44
1:A:249:VAL:HB	1:A:273:GLU:OE2	2.17	0.44
1:A:416:LEU:HD11	1:C:397:GLN:HG3	2.00	0.44
1:C:306:ALA:CB	1:C:383:ARG:HG3	2.47	0.43
1:A:243:PHE:O	1:A:244:SER:HB3	2.18	0.43
1:A:395:LEU:HD23	1:A:395:LEU:HA	1.80	0.43
1:C:238:CYS:HA	1:C:241:ARG:HD3	2.00	0.43
1:C:309:ILE:HG23	1:C:310:GLU:N	2.33	0.42
1:C:250:THR:HA	1:C:251:PRO:HD3	1.76	0.42
1:C:425:LEU:O	1:C:429:ARG:HG2	2.19	0.42
1:A:411:ARG:HD3	1:A:417:ARG:CD	2.50	0.42
1:C:297:ARG:HD3	1:C:297:ARG:O	2.20	0.42
1:C:430:THR:O	1:C:434:VAL:HG23	2.20	0.42
1:C:410:LYS:HG3	1:C:411:ARG:HG3	2.00	0.42
1:C:323:GLU:HA	1:C:323:GLU:OE1	2.20	0.42
1:A:236:LEU:HG	1:A:240:LYS:HE3	2.02	0.41
1:C:407:THR:HG21	1:C:421:MET:CE	2.50	0.41
1:C:409:ILE:HG22	1:C:410:LYS:N	2.36	0.41
1:C:279:VAL:O	1:C:283:VAL:HG23	2.20	0.41
1:C:236:LEU:HG	1:C:237:GLN:N	2.35	0.41
1:C:346:GLN:O	1:C:350:ILE:HG13	2.20	0.41
1:C:455:GLU:HG3	2:D:366:HIS:HA	2.01	0.41
1:C:346:GLN:HG3	1:C:348:GLU:CD	2.41	0.41
1:A:283:VAL:HA	1:A:304:LEU:HD21	2.03	0.41
1:A:414:ASP:C	1:A:416:LEU:H	2.23	0.41
1:A:451:PRO:O	1:A:455:GLU:N	2.52	0.41
1:C:252:TRP:HA	1:C:253:PRO:HD3	1.87	0.41
1:C:365:LEU:HA	1:C:369:GLU:OE1	2.20	0.41
1:C:424:LYS:HD3	1:C:424:LYS:HA	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:ARG:HB3	1:C:444:LEU:HD23	2.01	0.41
1:C:397:GLN:N	1:C:398:PRO:HD2	2.35	0.41
1:C:306:ALA:HB3	1:C:383:ARG:HG3	2.03	0.40
1:C:315:GLU:O	1:C:319:ARG:HG2	2.21	0.40
1:A:401:GLU:HG3	1:C:415:GLN:NE2	2.37	0.40
1:C:340:PHE:O	1:C:345:LEU:HD13	2.21	0.40
1:A:429:ARG:HA	1:A:429:ARG:HD3	1.89	0.40
1:A:443:ARG:O	1:A:445:GLN:N	2.54	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	227/247 (92%)	207 (91%)	18 (8%)	2 (1%)	20	49
1	C	223/247 (90%)	207 (93%)	14 (6%)	2 (1%)	20	49
2	B	10/12 (83%)	8 (80%)	2 (20%)	0	100	100
2	D	10/12 (83%)	10 (100%)	0	0	100	100
All	All	470/518 (91%)	432 (92%)	34 (7%)	4 (1%)	20	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	446	ASP
1	C	364	GLY
1	A	330	LEU
1	A	444	LEU

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	208/219 (95%)	196 (94%)	12 (6%)	23	52
1	C	204/219 (93%)	189 (93%)	15 (7%)	16	38
2	B	12/12 (100%)	12 (100%)	0	100	100
2	D	12/12 (100%)	11 (92%)	1 (8%)	13	33
All	All	436/462 (94%)	408 (94%)	28 (6%)	20	47

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	GLN
1	A	261	ARG
1	A	298	GLU
1	A	304	LEU
1	A	361	ARG
1	A	377	ASN
1	A	387	GLN
1	A	401	GLU
1	A	421	MET
1	A	436	SER
1	A	437	GLU
1	A	444	LEU
1	C	236	LEU
1	C	262	ASP
1	C	265	GLN
1	C	278	SER
1	C	280	GLN
1	C	307	SER
1	C	333	PHE
1	C	342	ARG
1	C	346	GLN
1	C	383	ARG
1	C	417	ARG
1	C	443	ARG

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Mol	Chain	Res	Type
1	C	444	LEU
1	C	448	LYS
1	C	455	GLU
2	D	367	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	239	ASN
1	A	266	GLN
1	A	377	ASN
1	A	413	GLN
1	A	435	HIS
1	C	230	GLN
1	C	235	GLN
1	C	265	GLN
1	C	266	GLN
1	C	280	GLN
1	C	288	GLN
1	C	294	GLN
1	C	435	HIS
1	C	445	GLN
2	D	367	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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	0KT	A	501	-	32,34,34	2.94	4 (12%)	44,51,51	2.41	4 (9%)
4	ACT	A	502	5	1,3,3	3.05	1 (100%)	0,3,3	0.00	-
3	0KT	C	501	-	32,34,34	2.66	5 (15%)	44,51,51	2.51	6 (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
3	0KT	A	501	-	-	0/35/41/41	0/3/3/3
4	ACT	A	502	5	-	0/0/0/0	0/0/0/0
3	0KT	C	501	-	-	0/35/41/41	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	0KT	C3-C1	2.01	1.42	1.39
3	A	501	0KT	C10-C8	2.08	1.42	1.38
3	C	501	0KT	C10-C8	2.45	1.42	1.38
3	C	501	0KT	C2-C1	2.47	1.43	1.39
3	A	501	0KT	C2-C1	2.69	1.43	1.39
3	A	501	0KT	C20-C18	2.91	1.58	1.54
4	A	502	ACT	CH3-C	3.05	1.52	1.48
3	C	501	0KT	C20-C18	5.87	1.61	1.54
3	C	501	0KT	S2-N1	11.84	1.77	1.64
3	A	501	0KT	S2-N1	14.83	1.80	1.64

All (10) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	0KT	C7-N1-C6	-13.83	104.51	117.02
3	A	501	0KT	C7-N1-C6	-13.12	105.16	117.02
3	C	501	0KT	O4-S2-N1	-2.53	104.26	106.81
3	A	501	0KT	O4-S2-N1	-2.38	104.40	106.81
3	C	501	0KT	C7-N1-S2	-2.20	113.67	117.20
3	C	501	0KT	C17-C16-N2	2.10	110.42	107.57
3	A	501	0KT	C15-N2-C19	3.41	130.44	124.72
3	C	501	0KT	C15-N2-C19	3.50	130.60	124.72
3	C	501	0KT	C8-S2-N1	6.19	114.67	106.75
3	A	501	0KT	C8-S2-N1	6.36	114.89	106.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	0KT	3	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(Å²)	Q<0.9
1	A	233/247 (94%)	0.15	10 (4%)	36	30	55, 75, 123, 139	0
1	C	229/247 (92%)	0.21	9 (3%)	40	34	53, 87, 129, 144	0
2	B	12/12 (100%)	0.51	0	100	100	87, 99, 113, 115	0
2	D	12/12 (100%)	-0.36	0	100	100	64, 73, 89, 100	0
All	All	486/518 (93%)	0.17	19 (3%)	40	34	53, 79, 126, 144	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	LEU	5.1
1	A	331	LYS	4.0
1	C	241	ARG	3.8
1	A	251	PRO	3.1
1	A	248	LYS	3.1
1	C	331	LYS	3.1
1	C	253	PRO	2.9
1	C	349	PHE	2.8
1	C	329	PHE	2.7
1	A	332	ASP	2.6
1	C	346	GLN	2.6
1	A	307	SER	2.6
1	A	288	GLN	2.4
1	A	312	MET	2.3
1	C	342	ARG	2.2
1	A	218	MET	2.2
1	A	308	THR	2.2
1	C	240	LYS	2.1
1	C	345	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
5	CA	C	502	1/1	0.97	0.42	3.64	103,103,103,103	0
5	CA	A	503	1/1	0.83	0.41	3.26	124,124,124,124	0
3	0KT	A	501	32/32	0.86	0.33	2.59	78,88,100,104	0
3	0KT	C	501	32/32	0.88	0.34	1.88	113,118,127,127	0
5	CA	A	505	1/1	0.80	0.20	-	73,73,73,73	1
5	CA	A	504	1/1	0.69	0.36	-	126,126,126,126	0
5	CA	C	503	1/1	0.85	0.24	-	126,126,126,126	0
4	ACT	A	502	4/4	0.82	0.35	-	99,99,100,101	0
5	CA	A	506	1/1	0.91	0.38	-	105,105,105,105	1

6.5 Other polymers ⓘ

There are no such residues in this entry.