



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:49 PM GMT

PDB ID : 4DK7  
Title : Crystal structure of LXR ligand binding domain in complex with full agonist 1  
Authors : Piper, D.E.; Xu, H.  
Deposited on : 2012-02-03  
Resolution : 2.45 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

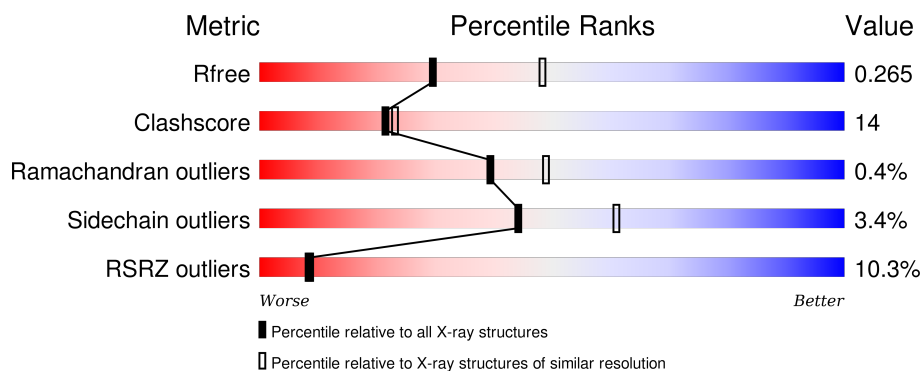
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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  $\geq 3$ , 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	247	<div> <div>7%</div> <div>73%</div> <div>21%</div> <div>• 5%</div> </div>
1	C	247	<div> <div>12%</div> <div>61%</div> <div>30%</div> <div>• 7%</div> </div>
2	B	12	<div> <div>8%</div> <div>58%</div> <div>42%</div> </div>
2	D	12	<div> <div>8%</div> <div>67%</div> <div>33%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	0KS	A	501	-	-	-	X
3	0KS	C	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 4178 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	235	Total	C	N	O	S	Se	0	0	0
			1921	1229	339	345	2	6			
1	C	229	Total	C	N	O	S	Se	0	0	0
			1870	1199	328	336	2	5			

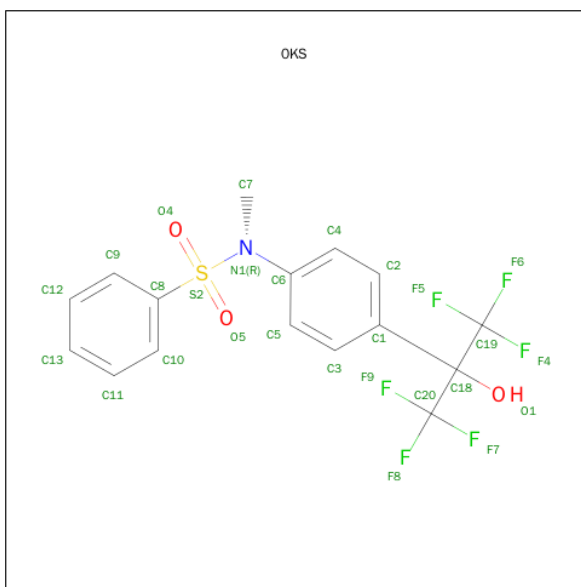
There are 8 discrepancies between the modelled and reference sequences:

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	MSE	-	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	MSE	-	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	C	N	O	0	0	0
			108	68	19	21			
2	D	12	Total	C	N	O	0	0	0
			108	68	19	21			

- Molecule 3 is N-[4-(1,1,1,3,3,3-HEXAFLUORO-2-HYDROXYPROPAN-2-YL)PHENYL]-N-METHYLBENZENESULFONAMIDE (three-letter code: 0KS) (formula: C<sub>16</sub>H<sub>13</sub>F<sub>6</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			27	16	6	1	3	1		
3	C	1	Total	C	F	N	O	S	0	0
			27	16	6	1	3	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	5	Total Ca 5 5	0	0
5	C	2	Total Ca 2 2	0	0

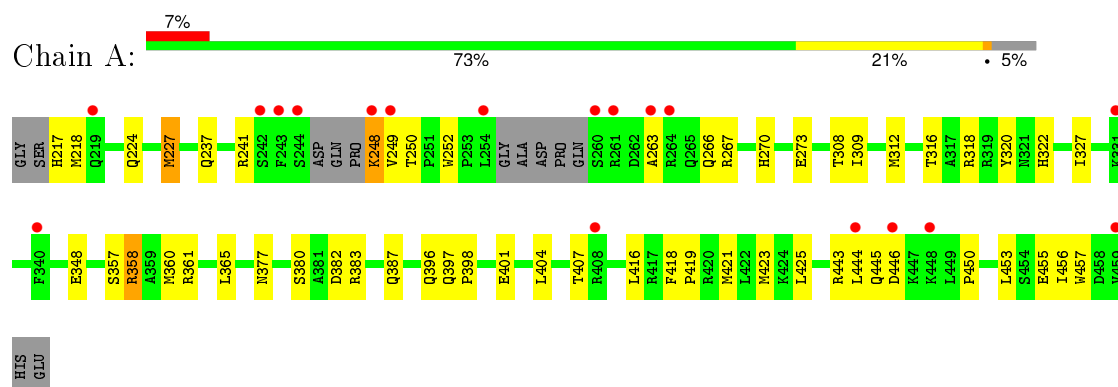
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	61	Total O 61 61	0	0
6	B	1	Total O 1 1	0	0
6	C	37	Total O 37 37	0	0
6	D	7	Total O 7 7	0	0

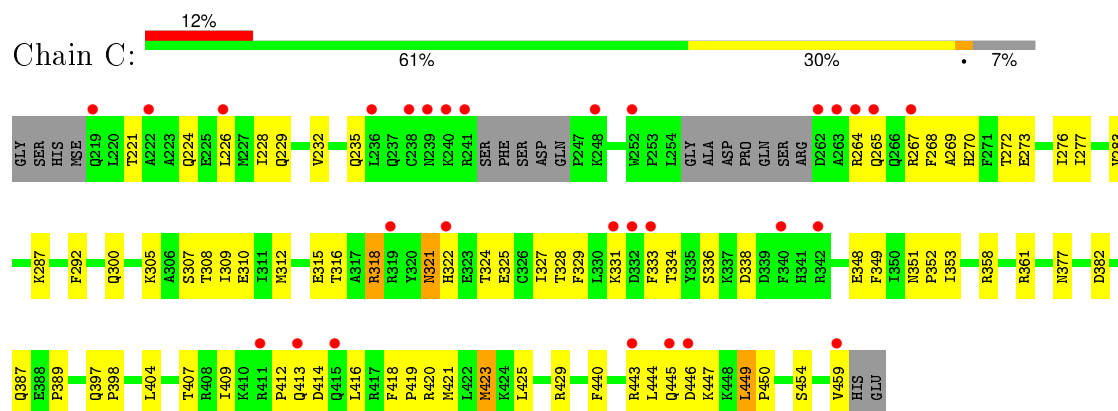
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Oxysterols receptor LXR-beta



#### • Molecule 1: Oxysterols receptor LXR-beta



#### • Molecule 2: Nuclear receptor coactivator 1



#### • Molecule 2: Nuclear receptor coactivator 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.26 Å 87.26 Å 197.71 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 19.96 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.45) 99.9 (19.96-2.45)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.47 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.230 , 0.270 0.226 , 0.265	Depositor DCC
$R_{free}$ test set	1456 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.7	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 28711 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0KS, CA, 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	0.36	0/1951	0.49	0/2624
1	C	0.32	0/1900	0.49	0/2559
2	B	0.33	0/109	0.44	0/144
2	D	0.40	0/109	0.44	0/144
All	All	0.34	0/4069	0.49	0/5471

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 [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	1921	0	1953	52	0
1	C	1870	0	1908	62	0
2	B	108	0	105	5	0
2	D	108	0	105	4	0
3	A	27	0	13	0	0
3	C	27	0	13	2	0
4	A	4	0	3	0	0
5	A	5	0	0	0	0
5	C	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	61	0	0	0	0
6	B	1	0	0	0	0
6	C	37	0	0	3	0
6	D	7	0	0	0	0
All	All	4178	0	4100	115	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 14.

All (115) 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:449:LEU:HD12	1:C:449:LEU:H	1.39	0.85
1:A:312:MSE:HE1	1:A:457:TRP:CZ2	2.17	0.79
1:A:419:PRO:O	1:A:423:MSE:HG2	1.84	0.77
1:A:308:THR:HG22	1:A:312:MSE:HE2	1.67	0.76
1:A:407:THR:HG21	1:A:421:MSE:HE1	1.66	0.76
1:A:418:PHE:HB3	1:A:419:PRO:HD3	1.68	0.75
1:A:312:MSE:HE1	1:A:457:TRP:HZ2	1.52	0.75
1:A:308:THR:HG22	1:A:312:MSE:CE	2.21	0.70
1:C:443:ARG:HH12	1:C:459:VAL:H	1.38	0.69
1:A:396:GLN:OE1	1:C:423:MSE:HE1	1.93	0.68
1:C:328:THR:HG22	1:C:334:THR:HG22	1.74	0.68
1:C:224:GLN:O	1:C:228:ILE:HG13	1.94	0.67
1:C:272:THR:O	1:C:276:ILE:HG13	1.93	0.67
1:A:416:LEU:C	1:A:419:PRO:HD2	2.16	0.67
1:C:409:ILE:O	1:C:412:PRO:HD3	1.95	0.66
1:C:418:PHE:HB3	1:C:419:PRO:HD3	1.78	0.65
2:D:375:LYS:O	2:D:376:ASP:HB2	1.97	0.65
1:A:217:HIS:CE1	1:A:218:MSE:HG2	2.32	0.64
1:C:440:PHE:O	1:C:443:ARG:HB2	1.99	0.62
1:C:269:ALA:O	1:C:273:GLU:HG3	2.00	0.62
1:C:351:ASN:HB2	1:C:352:PRO:HD3	1.82	0.62
1:A:423:MSE:HA	1:A:423:MSE:HE2	1.84	0.60
1:C:420:ARG:HA	1:C:423:MSE:HG3	1.84	0.59
1:C:228:ILE:O	1:C:232:VAL:HG23	2.02	0.59
1:A:377:ASN:HD22	1:A:425:LEU:HD22	1.68	0.59
1:C:429:ARG:HD3	6:C:613:HOH:O	2.02	0.59
1:A:407:THR:HG21	1:A:421:MSE:CE	2.32	0.59
1:C:312:MSE:HE2	3:C:501:OKS:H4	1.87	0.57
1:A:250:THR:N	1:A:273:GLU:OE1	2.37	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:THR:HG22	1:C:421:MSE:HE1	1.88	0.56
1:A:252:TRP:CZ2	1:A:267:ARG:HD3	2.41	0.56
3:C:501:0KS:H7	6:C:637:HOH:O	2.06	0.56
1:A:357:SER:O	1:A:361:ARG:HG2	2.06	0.55
1:C:321:ASN:HD22	1:C:322:HIS:N	2.04	0.55
1:C:328:THR:HA	1:C:333:PHE:O	2.05	0.55
1:A:404:LEU:HD13	1:A:418:PHE:CD2	2.42	0.55
1:C:307:SER:HB2	1:C:377:ASN:OD1	2.08	0.54
1:A:416:LEU:O	1:A:419:PRO:HD2	2.08	0.54
1:C:349:PHE:O	1:C:353:ILE:HG13	2.07	0.54
1:C:449:LEU:HD12	1:C:449:LEU:N	2.14	0.53
2:B:372:LEU:HD23	2:B:375:LYS:HE3	1.90	0.53
1:A:248:LYS:HD2	1:A:249:VAL:N	2.23	0.53
2:D:375:LYS:O	2:D:376:ASP:CB	2.58	0.52
1:C:292:PHE:CE2	1:C:300:GLN:HG2	2.44	0.51
1:A:418:PHE:HA	1:A:421:MSE:CE	2.41	0.51
1:C:443:ARG:NH1	1:C:459:VAL:H	2.08	0.51
1:C:407:THR:CG2	1:C:421:MSE:HE1	2.41	0.50
1:A:249:VAL:HB	1:A:273:GLU:OE1	2.11	0.50
1:C:382:ASP:CG	1:C:429:ARG:HH22	2.15	0.50
1:A:443:ARG:C	1:A:445:GLN:H	2.16	0.49
1:C:273:GLU:O	1:C:277:ILE:HG13	2.13	0.49
1:A:252:TRP:CH2	1:A:267:ARG:HD3	2.48	0.48
1:C:316:THR:HG23	1:C:327:ILE:HG21	1.94	0.48
1:C:358:ARG:O	1:C:361:ARG:HB3	2.13	0.48
1:C:235:GLN:NE2	1:C:318:ARG:HH12	2.12	0.48
1:C:276:ILE:HD11	1:C:450:PRO:HG2	1.95	0.48
1:A:455:GLU:CG	2:B:366:HIS:HA	2.43	0.48
1:A:445:GLN:O	1:A:446:ASP:HB3	2.13	0.48
1:A:419:PRO:HG3	1:C:418:PHE:HE2	1.78	0.47
1:C:221:THR:OG1	1:C:224:GLN:HG3	2.14	0.47
1:C:349:PHE:CZ	1:C:353:ILE:HD11	2.49	0.47
1:C:416:LEU:C	1:C:419:PRO:HD2	2.34	0.47
1:A:224:GLN:HA	1:A:227:MSE:HE3	1.97	0.47
1:A:312:MSE:HE1	1:A:457:TRP:CH2	2.48	0.47
1:A:416:LEU:HD11	1:C:397:GLN:HG3	1.96	0.46
1:A:316:THR:CG2	1:A:327:ILE:HD13	2.45	0.46
1:A:309:ILE:HA	1:A:312:MSE:HE3	1.96	0.46
1:C:404:LEU:HD13	1:C:418:PHE:CD2	2.51	0.46
1:C:444:LEU:C	1:C:446:ASP:H	2.19	0.46
1:A:263:ALA:O	1:A:267:ARG:HG3	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:CG1	1:A:273:GLU:HB3	2.45	0.45
1:C:449:LEU:HD13	1:C:454:SER:HB2	1.98	0.45
1:C:226:LEU:HA	1:C:229:GLN:NE2	2.31	0.45
1:A:456:ILE:HD11	2:B:369:LEU:HD22	1.98	0.45
1:C:419:PRO:O	1:C:423:MSE:HG2	2.17	0.45
1:A:360:MSE:HE1	1:A:365:LEU:HD11	1.99	0.45
1:C:305:LYS:HD2	2:D:366:HIS:NE2	2.31	0.45
1:C:382:ASP:OD2	1:C:429:ARG:NH2	2.49	0.45
1:C:315:GLU:HA	1:C:315:GLU:OE2	2.16	0.45
1:A:320:TYR:CE2	1:A:322:HIS:HA	2.53	0.44
1:C:283:VAL:O	1:C:287:LYS:HG3	2.18	0.44
1:A:418:PHE:HE2	1:C:419:PRO:HG3	1.82	0.44
1:C:235:GLN:CD	1:C:318:ARG:HH12	2.20	0.44
1:A:456:ILE:CD1	2:B:369:LEU:HD22	2.48	0.44
2:D:366:HIS:O	2:D:370:ARG:HG3	2.17	0.44
1:A:380:SER:O	1:A:383:ARG:HG2	2.18	0.44
1:A:423:MSE:HE1	1:C:425:LEU:HD12	2.00	0.43
1:A:397:GLN:N	1:A:398:PRO:HD2	2.33	0.43
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.84	0.43
1:C:348:GLU:O	1:C:352:PRO:HG2	2.17	0.43
1:A:360:MSE:HE1	1:A:365:LEU:CD1	2.48	0.43
1:A:250:THR:HG21	1:A:266:GLN:HG3	2.00	0.43
1:A:237:GLN:HG2	1:A:241:ARG:HH11	1.84	0.43
1:C:387:GLN:C	1:C:389:PRO:HD3	2.39	0.43
1:A:267:ARG:O	1:A:270:HIS:HB3	2.19	0.43
1:C:309:ILE:HG23	1:C:310:GLU:N	2.34	0.43
1:C:449:LEU:H	1:C:449:LEU:CD1	2.12	0.42
2:B:375:LYS:O	2:B:376:ASP:HB2	2.19	0.42
1:C:308:THR:HG22	1:C:309:ILE:N	2.34	0.42
1:A:443:ARG:C	1:A:445:GLN:N	2.72	0.42
1:A:450:PRO:HD2	1:A:453:LEU:HD12	2.02	0.42
1:A:397:GLN:O	1:A:401:GLU:HG3	2.19	0.42
1:C:387:GLN:HG2	6:C:624:HOH:O	2.18	0.42
1:C:413:GLN:HG3	1:C:414:ASP:H	1.85	0.42
1:C:459:VAL:HG12	1:C:459:VAL:O	2.19	0.42
1:A:453:LEU:HD22	1:A:457:TRP:CZ3	2.55	0.42
1:A:456:ILE:HG22	1:A:457:TRP:CD1	2.55	0.42
1:C:229:GLN:HB2	1:C:229:GLN:HE21	1.69	0.41
1:C:226:LEU:HA	1:C:229:GLN:HE21	1.86	0.41
1:C:336:SER:C	1:C:338:ASP:N	2.74	0.41
1:A:418:PHE:HA	1:A:421:MSE:HE3	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:GLN:N	1:C:398:PRO:HD2	2.36	0.41
1:C:324:THR:O	1:C:325:GLU:HB2	2.22	0.40
1:C:268:PHE:CD2	1:C:447:LYS:HD2	2.56	0.40
1:C:267:ARG:O	1:C:270:HIS:HB3	2.21	0.40

There are no symmetry-related clashes.

## 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	229/247 (93%)	226 (99%)	2 (1%)	1 (0%)	39	49
1	C	223/247 (90%)	217 (97%)	5 (2%)	1 (0%)	39	49
2	B	10/12 (83%)	10 (100%)	0	0	100	100
2	D	10/12 (83%)	10 (100%)	0	0	100	100
All	All	472/518 (91%)	463 (98%)	7 (2%)	2 (0%)	39	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	LEU
1	C	445	GLN

### 5.3.2 Protein sidechains [i](#)

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	210/213 (99%)	203 (97%)	7 (3%)	45	61
1	C	204/213 (96%)	196 (96%)	8 (4%)	39	54
2	B	12/12 (100%)	12 (100%)	0	100	100
2	D	12/12 (100%)	12 (100%)	0	100	100
All	All	438/450 (97%)	423 (97%)	15 (3%)	44	61

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	MSE
1	A	248	LYS
1	A	318	ARG
1	A	348	GLU
1	A	358	ARG
1	A	382	ASP
1	A	387	GLN
1	C	264	ARG
1	C	265	GLN
1	C	318	ARG
1	C	321	ASN
1	C	329	PHE
1	C	331	LYS
1	C	423	MSE
1	C	449	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	265	GLN
1	A	351	ASN
1	A	377	ASN
1	C	224	GLN
1	C	229	GLN
1	C	237	GLN
1	C	265	GLN
1	C	321	ASN
1	C	341	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 7 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	OKS	A	501	-	28,28,28	1.89	7 (25%)	42,45,45	1.40	5 (11%)
4	ACT	A	502	5	1,3,3	2.56	1 (100%)	0,3,3	0.00	-
3	OKS	C	501	-	28,28,28	2.05	7 (25%)	42,45,45	1.46	5 (11%)

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	OKS	A	501	-	-	0/40/40/40	0/2/2/2
4	ACT	A	502	5	-	0/0/0/0	0/0/0/0
3	OKS	C	501	-	-	0/40/40/40	0/2/2/2

All (15) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	OKS	C3-C1	2.04	1.42	1.39
3	C	501	OKS	C9-C8	2.15	1.42	1.38
3	C	501	OKS	C5-C6	2.33	1.43	1.39
3	C	501	OKS	C10-C8	2.36	1.42	1.38
3	C	501	OKS	C19-C18	2.36	1.59	1.54
3	A	501	OKS	C2-C1	2.36	1.42	1.39
3	A	501	OKS	C9-C8	2.56	1.43	1.38
4	A	502	ACT	CH3-C	2.56	1.52	1.48
3	A	501	OKS	C10-C8	2.59	1.43	1.38
3	C	501	OKS	C2-C1	2.63	1.43	1.39
3	A	501	OKS	C20-C18	2.68	1.59	1.54
3	A	501	OKS	C8-S2	2.80	1.80	1.76
3	C	501	OKS	C20-C18	4.08	1.62	1.54
3	A	501	OKS	S2-N1	5.93	1.77	1.65
3	C	501	OKS	S2-N1	6.32	1.77	1.65

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	OKS	C7-N1-S2	-4.78	110.64	117.79
3	A	501	OKS	C7-N1-S2	-4.63	110.87	117.79
3	C	501	OKS	O5-S2-O4	-2.65	114.89	119.47
3	A	501	OKS	O5-S2-O4	-2.25	115.58	119.47
3	A	501	OKS	C6-N1-S2	2.55	122.36	116.63
3	C	501	OKS	C6-N1-S2	2.76	122.83	116.63
3	A	501	OKS	C8-S2-N1	3.40	111.28	106.58
3	C	501	OKS	C8-S2-N1	3.59	111.54	106.58
3	A	501	OKS	C20-C18-C19	4.76	114.70	110.55
3	C	501	OKS	C20-C18-C19	4.96	114.88	110.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	OKS	2	0

## 5.7 Other polymers ⓘ

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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	229/247 (92%)	0.23	18 (7%) 15 16	39, 57, 96, 116	0
1	C	224/247 (90%)	0.50	29 (12%) 5 4	35, 72, 108, 131	0
2	B	12/12 (100%)	0.33	1 (8%) 14 14	63, 73, 86, 86	0
2	D	12/12 (100%)	-0.01	1 (8%) 14 14	47, 54, 76, 86	0
All	All	477/518 (92%)	0.35	49 (10%) 9 8	35, 61, 106, 131	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	PHE	6.5
1	A	242	SER	5.4
1	A	261	ARG	5.0
1	C	239	ASN	4.5
1	C	263	ALA	4.4
1	C	241	ARG	4.3
1	C	240	LYS	4.1
1	A	260	SER	4.1
1	A	459	VAL	4.0
1	C	332	ASP	3.9
1	A	446	ASP	3.7
1	C	443	ARG	3.6
1	C	238	CYS	3.6
1	A	264	ARG	3.5
1	C	342	ARG	3.4
1	C	236	LEU	3.3
1	A	248	LYS	3.2
1	C	446	ASP	3.2
1	A	254	LEU	3.1
1	C	226	LEU	3.1
1	C	331	LYS	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	413	GLN	3.0
2	D	376	ASP	2.9
1	C	264	ARG	2.8
1	C	252	TRP	2.8
1	C	333	PHE	2.8
1	A	244	SER	2.8
1	C	340	PHE	2.8
1	C	322	HIS	2.8
1	C	262	ASP	2.7
1	C	411	ARG	2.7
1	A	331	LYS	2.7
1	C	222	ALA	2.5
1	C	459	VAL	2.5
1	A	444	LEU	2.4
1	A	448	LYS	2.3
1	A	408	ARG	2.3
1	C	219	GLN	2.3
1	A	249	VAL	2.2
1	C	415	GLN	2.2
1	A	219	GLN	2.1
2	B	376	ASP	2.1
1	C	265	GLN	2.1
1	A	263	ALA	2.1
1	C	267	ARG	2.1
1	A	340	PHE	2.1
1	C	445	GLN	2.0
1	C	319	ARG	2.0
1	C	248	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	CA	C	502	1/1	0.95	0.46	7.77	105,105,105,105	0
3	OKS	A	501	27/27	0.85	0.33	3.58	52,62,81,82	0
3	OKS	C	501	27/27	0.86	0.34	3.16	87,95,105,106	0
5	CA	A	503	1/1	0.97	0.20	2.80	92,92,92,92	0
5	CA	A	505	1/1	0.99	0.17	-	70,70,70,70	1
5	CA	A	506	1/1	0.86	0.37	-	104,104,104,104	1
5	CA	A	507	1/1	0.73	0.46	-	90,90,90,90	1
4	ACT	A	502	4/4	0.79	0.20	-	75,77,78,79	0
5	CA	C	503	1/1	0.53	0.19	-	142,142,142,142	0
5	CA	A	504	1/1	0.88	0.26	-	118,118,118,118	0

## 6.5 Other polymers

There are no such residues in this entry.