



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 03:07 am BST

PDB ID : 6JIO
Title : Human LXR-beta in complex with a ligand
Authors : Zhang, Z.; Zhou, H.
Deposited on : 2019-02-22
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

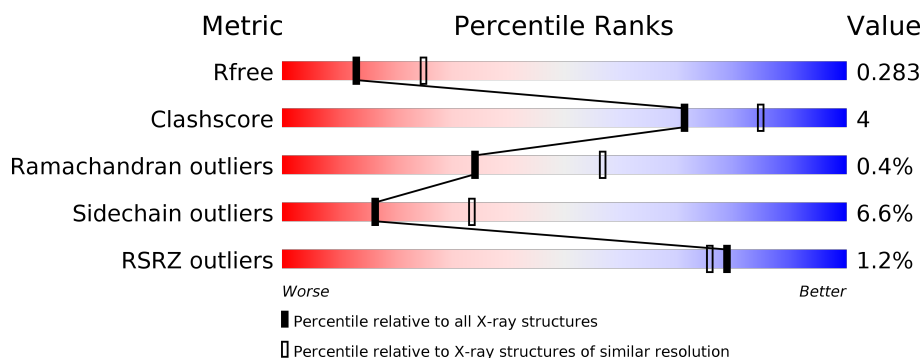
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	274	<div> <div></div> <div>79% 9% • 11%</div> </div>
1	B	274	<div> <div>%</div> <div>80% 8% • 12%</div> </div>
1	C	274	<div> <div>2%</div> <div>77% 9% • 14%</div> </div>
1	D	274	<div> <div>%</div> <div>81% 7% • 10%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7594 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	244	Total	C	N	O	S	0	0	0
			1910	1224	330	349	7			
1	B	242	Total	C	N	O	S	0	0	0
			1885	1209	327	342	7			
1	C	237	Total	C	N	O	S	0	0	0
			1814	1165	313	329	7			
1	D	247	Total	C	N	O	S	0	0	0
			1913	1228	330	348	7			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	MET	-	initiating methionine	UNP P55055
A	208	GLY	-	expression tag	UNP P55055
A	209	HIS	-	expression tag	UNP P55055
A	210	HIS	-	expression tag	UNP P55055
A	211	HIS	-	expression tag	UNP P55055
A	212	HIS	-	expression tag	UNP P55055
A	213	HIS	-	expression tag	UNP P55055
A	214	HIS	-	expression tag	UNP P55055
A	259	ALA	GLN	engineered mutation	UNP P55055
A	261	GLY	ARG	engineered mutation	UNP P55055
A	262	SER	ASP	engineered mutation	UNP P55055
A	264	SER	ARG	engineered mutation	UNP P55055
A	462	GLY	-	expression tag	UNP P55055
A	463	SER	-	expression tag	UNP P55055
A	464	GLY	-	expression tag	UNP P55055
A	465	SER	-	expression tag	UNP P55055
A	466	GLY	-	expression tag	UNP P55055
A	467	SER	-	expression tag	UNP P55055
A	468	HIS	-	expression tag	UNP P55055
A	469	LYS	-	expression tag	UNP P55055
A	470	ILE	-	expression tag	UNP P55055

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Chain	Residue	Modelled	Actual	Comment	Reference
A	471	LEU	-	expression tag	UNP P55055
A	472	HIS	-	expression tag	UNP P55055
A	473	ARG	-	expression tag	UNP P55055
A	474	LEU	-	expression tag	UNP P55055
A	475	LEU	-	expression tag	UNP P55055
A	476	GLN	-	expression tag	UNP P55055
A	477	ASP	-	expression tag	UNP P55055
A	478	SER	-	expression tag	UNP P55055
A	479	SER	-	expression tag	UNP P55055
A	480	SER	-	expression tag	UNP P55055
B	207	MET	-	initiating methionine	UNP P55055
B	208	GLY	-	expression tag	UNP P55055
B	209	HIS	-	expression tag	UNP P55055
B	210	HIS	-	expression tag	UNP P55055
B	211	HIS	-	expression tag	UNP P55055
B	212	HIS	-	expression tag	UNP P55055
B	213	HIS	-	expression tag	UNP P55055
B	214	HIS	-	expression tag	UNP P55055
B	259	ALA	GLN	engineered mutation	UNP P55055
B	261	GLY	ARG	engineered mutation	UNP P55055
B	262	SER	ASP	engineered mutation	UNP P55055
B	264	SER	ARG	engineered mutation	UNP P55055
B	462	GLY	-	expression tag	UNP P55055
B	463	SER	-	expression tag	UNP P55055
B	464	GLY	-	expression tag	UNP P55055
B	465	SER	-	expression tag	UNP P55055
B	466	GLY	-	expression tag	UNP P55055
B	467	SER	-	expression tag	UNP P55055
B	468	HIS	-	expression tag	UNP P55055
B	469	LYS	-	expression tag	UNP P55055
B	470	ILE	-	expression tag	UNP P55055
B	471	LEU	-	expression tag	UNP P55055
B	472	HIS	-	expression tag	UNP P55055
B	473	ARG	-	expression tag	UNP P55055
B	474	LEU	-	expression tag	UNP P55055
B	475	LEU	-	expression tag	UNP P55055
B	476	GLN	-	expression tag	UNP P55055
B	477	ASP	-	expression tag	UNP P55055
B	478	SER	-	expression tag	UNP P55055
B	479	SER	-	expression tag	UNP P55055
B	480	SER	-	expression tag	UNP P55055
C	207	MET	-	initiating methionine	UNP P55055

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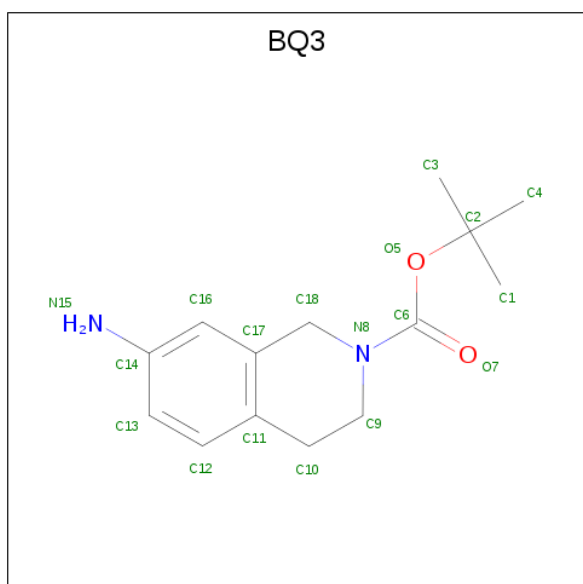
Chain	Residue	Modelled	Actual	Comment	Reference
C	208	GLY	-	expression tag	UNP P55055
C	209	HIS	-	expression tag	UNP P55055
C	210	HIS	-	expression tag	UNP P55055
C	211	HIS	-	expression tag	UNP P55055
C	212	HIS	-	expression tag	UNP P55055
C	213	HIS	-	expression tag	UNP P55055
C	214	HIS	-	expression tag	UNP P55055
C	259	ALA	GLN	engineered mutation	UNP P55055
C	261	GLY	ARG	engineered mutation	UNP P55055
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C	462	GLY	-	expression tag	UNP P55055
C	463	SER	-	expression tag	UNP P55055
C	464	GLY	-	expression tag	UNP P55055
C	465	SER	-	expression tag	UNP P55055
C	466	GLY	-	expression tag	UNP P55055
C	467	SER	-	expression tag	UNP P55055
C	468	HIS	-	expression tag	UNP P55055
C	469	LYS	-	expression tag	UNP P55055
C	470	ILE	-	expression tag	UNP P55055
C	471	LEU	-	expression tag	UNP P55055
C	472	HIS	-	expression tag	UNP P55055
C	473	ARG	-	expression tag	UNP P55055
C	474	LEU	-	expression tag	UNP P55055
C	475	LEU	-	expression tag	UNP P55055
C	476	GLN	-	expression tag	UNP P55055
C	477	ASP	-	expression tag	UNP P55055
C	478	SER	-	expression tag	UNP P55055
C	479	SER	-	expression tag	UNP P55055
C	480	SER	-	expression tag	UNP P55055
D	207	MET	-	initiating methionine	UNP P55055
D	208	GLY	-	expression tag	UNP P55055
D	209	HIS	-	expression tag	UNP P55055
D	210	HIS	-	expression tag	UNP P55055
D	211	HIS	-	expression tag	UNP P55055
D	212	HIS	-	expression tag	UNP P55055
D	213	HIS	-	expression tag	UNP P55055
D	214	HIS	-	expression tag	UNP P55055
D	259	ALA	GLN	engineered mutation	UNP P55055
D	261	GLY	ARG	engineered mutation	UNP P55055
D	262	SER	ASP	engineered mutation	UNP P55055
D	264	SER	ARG	engineered mutation	UNP P55055

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Chain	Residue	Modelled	Actual	Comment	Reference
D	462	GLY	-	expression tag	UNP P55055
D	463	SER	-	expression tag	UNP P55055
D	464	GLY	-	expression tag	UNP P55055
D	465	SER	-	expression tag	UNP P55055
D	466	GLY	-	expression tag	UNP P55055
D	467	SER	-	expression tag	UNP P55055
D	468	HIS	-	expression tag	UNP P55055
D	469	LYS	-	expression tag	UNP P55055
D	470	ILE	-	expression tag	UNP P55055
D	471	LEU	-	expression tag	UNP P55055
D	472	HIS	-	expression tag	UNP P55055
D	473	ARG	-	expression tag	UNP P55055
D	474	LEU	-	expression tag	UNP P55055
D	475	LEU	-	expression tag	UNP P55055
D	476	GLN	-	expression tag	UNP P55055
D	477	ASP	-	expression tag	UNP P55055
D	478	SER	-	expression tag	UNP P55055
D	479	SER	-	expression tag	UNP P55055
D	480	SER	-	expression tag	UNP P55055

- Molecule 2 is tert-butyl 7-amino-3,4-dihydroisoquinoline-2(1H)-carboxylate (three-letter code: BQ3) (formula: C₁₄H₂₀N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	14	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			18	14	2	2		

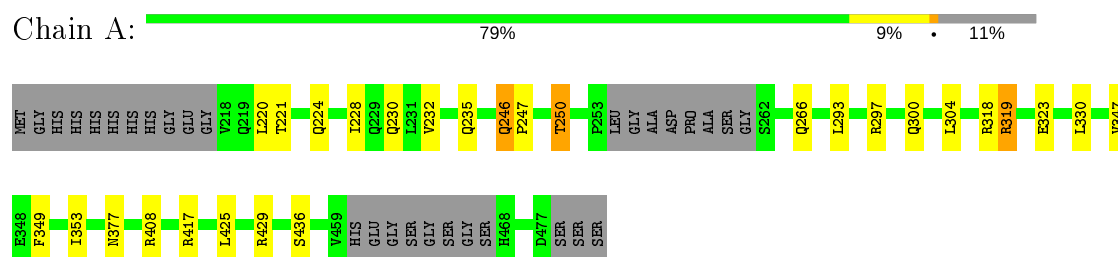
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	8	Total	O	0	0
			8	8		
3	C	6	Total	O	0	0
			6	6		
3	D	7	Total	O	0	0
			7	7		

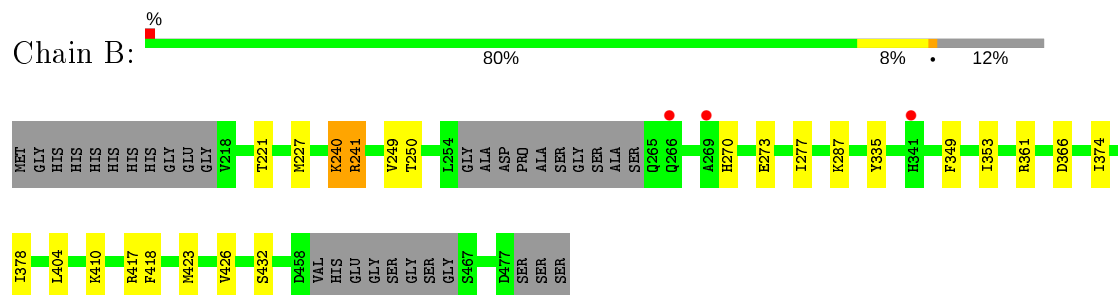
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

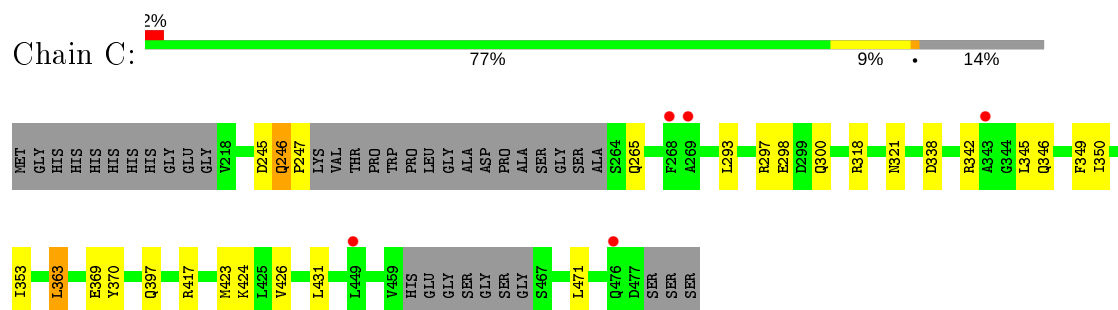
• Molecule 1: Oxysterols receptor LXR-beta



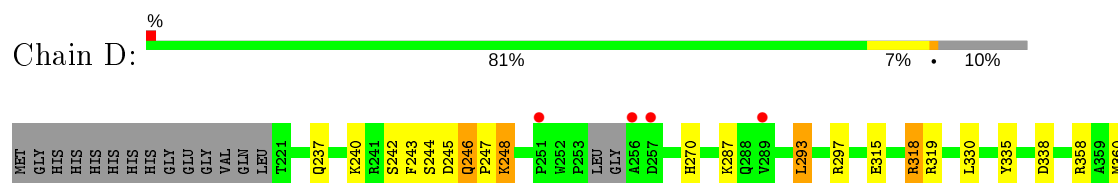
• Molecule 1: Oxysterols receptor LXR-beta



• Molecule 1: Oxysterols receptor LXR-beta



• Molecule 1: Oxysterols receptor LXR-beta



Q387	R391	Q397	V489	HIS	GLU	GLY	SER	GLY	SER	GLY	GLY	SER	H468	D477	SER	SER	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.14Å 106.89Å 150.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.60 50.14 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.01-2.60) 99.8 (50.14-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.262 , 0.285 0.262 , 0.283	Depositor DCC
R_{free} test set	1696 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7594	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: BQ3

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	0.38	0/1947	0.62	0/2644
1	B	0.37	0/1920	0.62	0/2607
1	C	0.37	0/1846	0.60	0/2508
1	D	0.38	0/1950	0.61	0/2647
All	All	0.38	0/7663	0.61	0/10406

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	1910	0	1862	13	0
1	B	1885	0	1841	12	0
1	C	1814	0	1742	8	0
1	D	1913	0	1873	20	0
2	A	18	0	0	0	0
2	D	18	0	0	0	0
3	A	15	0	0	0	0
3	B	8	0	0	0	0
3	C	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	7	0	0	0	0
All	All	7594	0	7318	52	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 4.

All (52) 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:B:241:ARG:HG3	1:B:241:ARG:HH11	1.03	1.09
1:B:241:ARG:CG	1:B:241:ARG:HH11	1.67	1.03
1:B:241:ARG:NH1	1:B:241:ARG:HG3	1.68	0.97
1:D:246:GLN:HG3	1:D:247:PRO:HD2	1.48	0.95
1:D:246:GLN:HB2	1:D:247:PRO:CD	2.00	0.92
1:D:246:GLN:CG	1:D:247:PRO:HD2	2.10	0.81
1:D:246:GLN:CB	1:D:247:PRO:CD	2.59	0.81
1:D:246:GLN:HB2	1:D:247:PRO:HD2	1.65	0.76
1:D:319:ARG:NH2	1:D:330:LEU:O	2.21	0.73
1:D:246:GLN:CB	1:D:247:PRO:HD2	2.19	0.73
1:A:250:THR:HG22	1:A:266:GLN:HE22	1.58	0.68
1:A:293:LEU:HA	1:A:300:GLN:HE22	1.61	0.65
1:B:270:HIS:HE2	1:B:335:TYR:HH	1.43	0.63
1:D:246:GLN:CG	1:D:247:PRO:CD	2.77	0.63
1:A:246:GLN:CB	1:A:247:PRO:CD	2.80	0.58
1:A:293:LEU:HA	1:A:300:GLN:NE2	2.18	0.58
1:D:246:GLN:HB2	1:D:247:PRO:HD3	1.85	0.58
1:B:270:HIS:NE2	1:B:335:TYR:OH	2.33	0.58
1:D:242:SER:CB	1:D:245:ASP:OD2	2.52	0.58
1:D:270:HIS:NE2	1:D:335:TYR:OH	2.26	0.58
1:C:246:GLN:CB	1:C:247:PRO:CD	2.85	0.55
1:D:246:GLN:HG3	1:D:247:PRO:CD	2.29	0.54
1:D:242:SER:HB3	1:D:245:ASP:OD2	2.08	0.53
1:D:287:LYS:O	1:D:293:LEU:HD11	2.10	0.52
1:A:349:PHE:CZ	1:A:353:ILE:HD11	2.45	0.51
1:D:315:GLU:OE1	1:D:318:ARG:NH1	2.43	0.51
1:D:242:SER:HB2	1:D:245:ASP:OD2	2.11	0.51
1:A:250:THR:CG2	1:A:266:GLN:HE22	2.23	0.50
1:A:377:ASN:HD22	1:A:425:LEU:HD22	1.76	0.50
1:D:245:ASP:O	1:D:246:GLN:O	2.30	0.49
1:A:228:ILE:O	1:A:232:VAL:HG13	2.14	0.48
1:C:349:PHE:CZ	1:C:353:ILE:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:GLN:CG	1:D:247:PRO:N	2.74	0.48
1:A:429:ARG:HG3	1:C:426:VAL:HG13	1.96	0.48
1:C:318:ARG:HD2	1:C:370:TYR:CG	2.49	0.47
1:A:377:ASN:HD22	1:A:425:LEU:CD2	2.28	0.46
1:B:273:GLU:O	1:B:277:ILE:HD12	2.16	0.46
1:D:243:PHE:O	1:D:248:LYS:NZ	2.49	0.45
1:B:366:ASP:OD2	1:B:410:LYS:NZ	2.51	0.44
1:C:369:GLU:OE2	1:C:417:ARG:NH2	2.51	0.44
1:A:232:VAL:HA	1:A:235:GLN:HG2	2.00	0.44
1:B:349:PHE:CZ	1:B:353:ILE:HD11	2.53	0.43
1:A:319:ARG:NH2	1:A:330:LEU:O	2.43	0.43
1:C:293:LEU:HA	1:C:300:GLN:NE2	2.34	0.43
1:B:240:LYS:H	1:B:240:LYS:HD2	1.84	0.42
1:B:404:LEU:HD13	1:B:418:PHE:CE2	2.54	0.42
1:B:374:ILE:O	1:B:378:ILE:HG13	2.19	0.42
1:C:318:ARG:HD2	1:C:370:TYR:CD2	2.55	0.42
1:C:363:LEU:O	1:C:417:ARG:NH1	2.52	0.42
1:D:358:ARG:CZ	1:D:358:ARG:HB3	2.50	0.42
1:B:241:ARG:NH1	1:B:241:ARG:CG	2.38	0.41
1:A:221:THR:HB	1:A:224:GLN:HG3	2.03	0.41

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	238/274 (87%)	234 (98%)	3 (1%)	1 (0%)	34	57
1	B	236/274 (86%)	231 (98%)	5 (2%)	0	100	100
1	C	231/274 (84%)	225 (97%)	4 (2%)	2 (1%)	17	35
1	D	241/274 (88%)	233 (97%)	7 (3%)	1 (0%)	34	57
All	All	946/1096 (86%)	923 (98%)	19 (2%)	4 (0%)	34	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	C	245	ASP
1	C	246	GLN
1	D	246	GLN

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	198/239 (83%)	186 (94%)	12 (6%)	18	38
1	B	194/239 (81%)	182 (94%)	12 (6%)	18	37
1	C	180/239 (75%)	165 (92%)	15 (8%)	11	22
1	D	197/239 (82%)	185 (94%)	12 (6%)	18	38
All	All	769/956 (80%)	718 (93%)	51 (7%)	16	33

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	LEU
1	A	230	GLN
1	A	250	THR
1	A	297	ARG
1	A	304	LEU
1	A	318	ARG
1	A	319	ARG
1	A	323	GLU
1	A	347	VAL
1	A	408	ARG
1	A	417	ARG
1	A	436	SER
1	B	221	THR
1	B	227	MET
1	B	240	LYS
1	B	241	ARG

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Mol	Chain	Res	Type
1	B	249	VAL
1	B	250	THR
1	B	287	LYS
1	B	361	ARG
1	B	417	ARG
1	B	423	MET
1	B	426	VAL
1	B	432	SER
1	C	265	GLN
1	C	297	ARG
1	C	298	GLU
1	C	321	ASN
1	C	338	ASP
1	C	342	ARG
1	C	345	LEU
1	C	346	GLN
1	C	350	ILE
1	C	363	LEU
1	C	397	GLN
1	C	423	MET
1	C	424	LYS
1	C	431	LEU
1	C	471	LEU
1	D	237	GLN
1	D	240	LYS
1	D	244	SER
1	D	248	LYS
1	D	293	LEU
1	D	297	ARG
1	D	318	ARG
1	D	338	ASP
1	D	360	MET
1	D	387	GLN
1	D	391	ARG
1	D	397	GLN

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

Mol	Chain	Res	Type
1	A	230	GLN
1	A	266	GLN
1	A	300	GLN

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Mol	Chain	Res	Type
1	A	377	ASN
1	A	435	HIS
1	C	280	GLN
1	C	321	ASN
1	C	397	GLN
1	D	235	GLN
1	D	321	ASN
1	D	472	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BQ3	A	501	-	19,19,19	0.30	0	27,28,28	0.49	0
2	BQ3	D	501	-	19,19,19	0.19	0	27,28,28	0.72	2 (7%)

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	BQ3	A	501	-	-	2/9/18/18	0/2/2/2
2	BQ3	D	501	-	-	5/9/18/18	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	BQ3	C18-N8-C9	-2.13	109.22	115.57
2	D	501	BQ3	O5-C2-C3	2.05	115.31	107.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	BQ3	N8-C6-O5-C2
2	D	501	BQ3	C4-C2-O5-C6
2	D	501	BQ3	C1-C2-O5-C6
2	D	501	BQ3	C3-C2-O5-C6
2	D	501	BQ3	O7-C6-O5-C2
2	A	501	BQ3	N8-C6-O5-C2
2	A	501	BQ3	O7-C6-O5-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	244/274 (89%)	-0.02	0 100 100	42, 68, 96, 116	0
1	B	242/274 (88%)	0.05	3 (1%) 79 76	43, 73, 155, 196	0
1	C	237/274 (86%)	0.14	5 (2%) 63 58	44, 72, 120, 131	0
1	D	247/274 (90%)	0.12	4 (1%) 72 68	49, 75, 121, 140	0
All	All	970/1096 (88%)	0.07	12 (1%) 79 76	42, 72, 120, 196	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	476	GLN	4.2
1	D	257	ASP	2.4
1	B	266	GLN	2.3
1	D	251	PRO	2.3
1	B	341	HIS	2.2
1	C	449	LEU	2.1
1	D	289	VAL	2.1
1	B	269	ALA	2.1
1	C	268	PHE	2.0
1	C	269	ALA	2.0
1	C	343	ALA	2.0
1	D	256	ALA	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 [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	BQ3	D	501	18/18	0.86	0.43	172,174,175,177	0
2	BQ3	A	501	18/18	0.90	0.45	172,174,176,176	0

6.5 Other polymers [i](#)

There are no such residues in this entry.