



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:35 am BST

PDB ID : 5Y49
Title : A moderator XD22 binding to bile acid receptor
Authors : Lu, Y.; Li, Y.
Deposited on : 2017-08-02
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

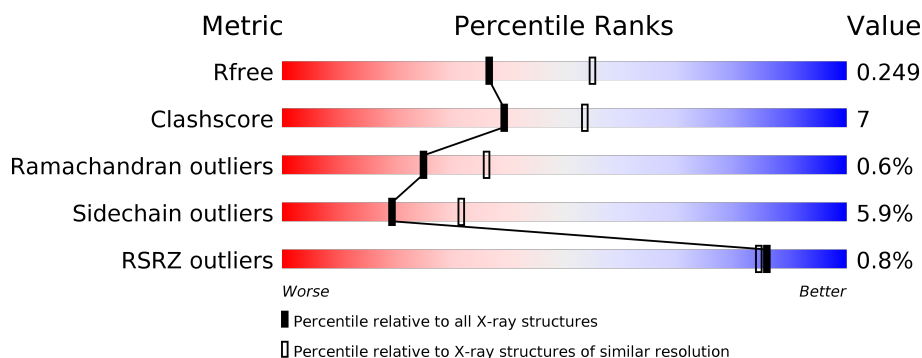
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	227	<div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	B	227	<div> <div>%</div> <div>83%</div> <div>15%</div> <div>• •</div> </div>
2	D	11	<div> <div>91%</div> <div>9%</div> </div>
2	E	11	<div> <div>55%</div> <div>27%</div> <div>9%</div> <div>9%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4030 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 Bile acid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1837	1174	308	344	11			
1	B	227	Total	C	N	O	S	0	0	0
			1863	1192	313	347	11			

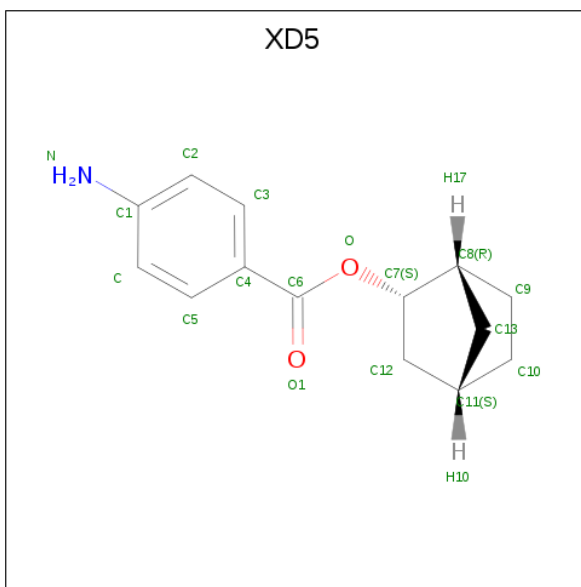
- Molecule 2 is a protein called Peptide from Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	0	0	0
			97	64	16	17			
2	E	10	Total	C	N	O	0	0	0
			85	55	14	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	688	LEU	ALA	conflict	UNP Q15596
E	688	LEU	ALA	conflict	UNP Q15596

- Molecule 3 is [(1R,2S,4S)-2-bicyclo[2.2.1]heptanyl] 4-azanylbenzoate (three-letter code: XD5) (formula: C₁₄H₁₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	17	0
			17	14	1	2		
3	B	1	Total	C	N	O	17	0
			17	14	1	2		

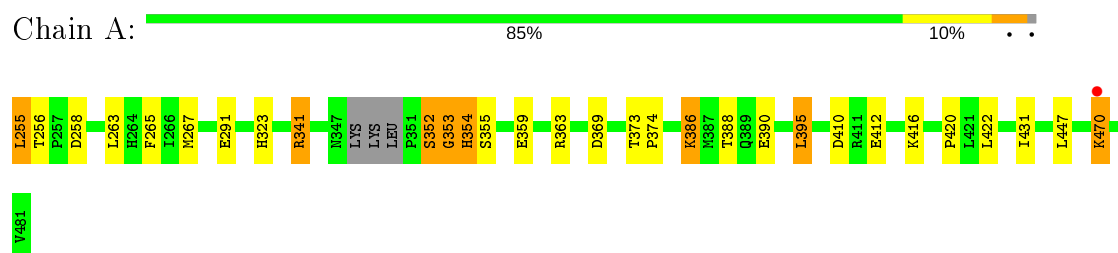
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	66	Total	O	0	0
			66	66		
4	D	1	Total	O	0	0
			1	1		
4	E	4	Total	O	0	0
			4	4		

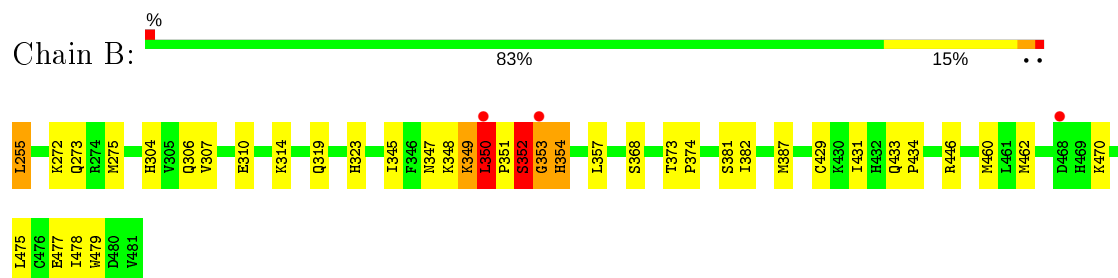
3 Residue-property plots [i](#)

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.

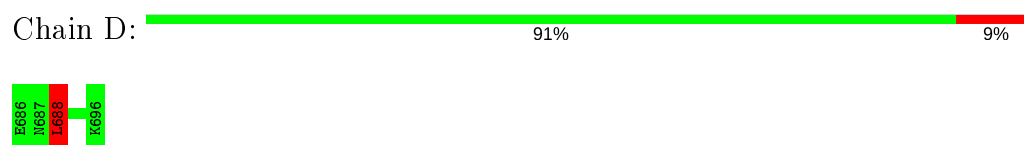
- Molecule 1: Bile acid receptor



- Molecule 1: Bile acid receptor



- Molecule 2: Peptide from Nuclear receptor coactivator 2



- Molecule 2: Peptide from Nuclear receptor coactivator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.81Å 34.85Å 117.31Å 90.00° 98.21° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 36.52 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.40) 96.2 (36.52-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135, REFMAC	Depositor
R, R_{free}	0.212 , 0.253 0.215 , 0.249	Depositor DCC
R_{free} test set	1116 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4030	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.20% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XD5

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	0.73	0/1876	0.88	3/2534 (0.1%)
1	B	0.82	0/1903	0.92	2/2571 (0.1%)
2	D	0.88	0/97	1.27	1/129 (0.8%)
2	E	1.24	1/85 (1.2%)	1.14	0/114
All	All	0.79	1/3961 (0.0%)	0.92	6/5348 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	686	GLU	CD-OE2	5.16	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	LEU	C-N-CD	-7.85	103.32	120.60
1	A	410	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	410	ASP	CB-CG-OD2	-6.44	112.50	118.30
2	D	688	LEU	CB-CG-CD1	5.88	121.00	111.00
1	A	341	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	460	MET	CA-CB-CG	5.24	122.20	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	GLY	Peptide

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	1837	0	1825	13	0
1	B	1863	0	1862	38	0
2	D	97	0	105	3	0
2	E	85	0	83	4	0
3	A	17	0	0	0	0
3	B	17	0	0	0	0
4	A	43	0	0	1	0
4	B	66	0	0	4	1
4	D	1	0	0	0	0
4	E	4	0	0	0	0
All	All	4030	0	3875	57	1

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 7.

All (57) 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:351:PRO:O	1:B:352:SER:HB3	1.40	1.14
1:A:352:SER:O	1:A:354:HIS:HB3	1.77	0.85
1:B:351:PRO:O	1:B:352:SER:CB	2.20	0.83
1:B:352:SER:OG	1:B:353:GLY:N	2.09	0.82
1:A:359:GLU:OE2	1:A:363:ARG:NH1	2.13	0.81
1:B:352:SER:O	1:B:354:HIS:N	2.17	0.77
1:B:350:LEU:HD13	1:B:350:LEU:O	1.83	0.77
1:B:349:LYS:O	1:B:351:PRO:CD	2.33	0.77
1:B:352:SER:C	1:B:354:HIS:H	1.84	0.76
1:B:349:LYS:O	1:B:351:PRO:HD3	1.87	0.74
1:A:352:SER:O	1:A:354:HIS:CB	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:LEU:HD22	1:B:479:TRP:CH2	2.28	0.69
1:B:477:GLU:OE1	4:B:601:HOH:O	2.12	0.67
1:B:352:SER:C	1:B:354:HIS:N	2.49	0.67
1:B:381:SER:HB3	1:B:446:ARG:HE	1.60	0.66
1:A:341:ARG:NH2	4:A:601:HOH:O	2.28	0.66
1:B:275:MET:HE2	1:B:345:ILE:HD13	1.80	0.64
1:B:314:LYS:HE3	4:B:609:HOH:O	1.98	0.64
1:B:273:GLN:HG3	4:B:658:HOH:O	2.01	0.61
1:B:353:GLY:O	1:B:357:LEU:HG	2.01	0.61
1:A:353:GLY:HA2	1:A:355:SER:H	1.66	0.60
2:D:688:LEU:HD22	2:D:688:LEU:H	1.66	0.60
1:B:349:LYS:O	1:B:351:PRO:HD2	2.01	0.58
1:B:349:LYS:N	1:B:349:LYS:HD2	2.19	0.58
2:D:688:LEU:N	2:D:688:LEU:HD22	2.19	0.57
1:B:345:ILE:HG12	1:B:349:LYS:HG2	1.88	0.55
1:B:319:GLN:HG2	4:B:627:HOH:O	2.09	0.53
1:B:349:LYS:C	1:B:351:PRO:HD3	2.28	0.53
1:A:395:LEU:HD12	1:A:447:LEU:HD21	1.91	0.52
1:B:431:ILE:O	1:B:434:PRO:HD3	2.09	0.52
2:E:686:GLU:O	2:E:686:GLU:CG	2.57	0.51
1:A:256:THR:HG22	1:A:258:ASP:N	2.26	0.51
1:B:347:ASN:C	1:B:350:LEU:HG	2.30	0.51
1:B:348:LYS:C	1:B:350:LEU:H	2.14	0.50
1:A:255:LEU:HD23	1:A:431:ILE:HD11	1.95	0.49
2:E:691:ARG:HD3	2:E:695:ASP:OD2	2.12	0.49
1:B:373:THR:HB	1:B:374:PRO:HD3	1.94	0.47
1:B:382:ILE:CD1	1:B:387:MET:HE1	2.45	0.47
1:B:446:ARG:HD3	1:B:446:ARG:HA	1.65	0.47
1:B:304:HIS:HE1	1:B:345:ILE:HD12	1.80	0.46
1:A:416:LYS:O	1:A:420:PRO:HD3	2.16	0.45
1:A:291:GLU:OE2	1:A:470:LYS:NZ	2.49	0.45
1:B:351:PRO:HB2	1:B:354:HIS:ND1	2.32	0.45
1:B:475:LEU:HD22	1:B:479:TRP:CZ3	2.51	0.44
1:B:382:ILE:HD13	1:B:387:MET:HE1	1.99	0.43
1:B:255:LEU:HG	1:B:431:ILE:HD11	2.01	0.43
1:B:429:CYS:O	1:B:433:GLN:HB2	2.19	0.43
2:E:686:GLU:O	2:E:686:GLU:HG3	2.18	0.43
1:B:477:GLU:OE2	2:E:687:ASN:HB3	2.18	0.43
2:D:688:LEU:HD13	2:D:688:LEU:H	1.84	0.43
1:B:306:GLN:O	1:B:310:GLU:HG2	2.19	0.42
1:B:348:LYS:HA	1:B:350:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:THR:HB	1:A:374:PRO:HD3	2.02	0.42
1:A:255:LEU:CD2	1:A:431:ILE:HD11	2.49	0.42
1:A:263:LEU:O	1:A:267:MET:HG2	2.19	0.41
1:B:273:GLN:HB3	1:B:307:VAL:HG13	2.01	0.41
1:B:350:LEU:HA	1:B:351:PRO:HD2	1.89	0.40

All (1) 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)
4:B:601:HOH:O	4:B:601:HOH:O[2_557]	2.04	0.16

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	220/227 (97%)	210 (96%)	9 (4%)	1 (0%)	29	41
1	B	225/227 (99%)	215 (96%)	8 (4%)	2 (1%)	17	25
2	D	9/11 (82%)	9 (100%)	0	0	100	100
2	E	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
All	All	462/476 (97%)	441 (96%)	18 (4%)	3 (1%)	25	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	352	SER
1	A	386	LYS
1	B	353	GLY

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	207/210 (99%)	194 (94%)	13 (6%)	18	28
1	B	210/210 (100%)	199 (95%)	11 (5%)	23	38
2	D	11/11 (100%)	10 (91%)	1 (9%)	9	14
2	E	9/11 (82%)	8 (89%)	1 (11%)	6	8
All	All	437/442 (99%)	411 (94%)	26 (6%)	19	32

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	LEU
1	A	265	PHE
1	A	323	HIS
1	A	352	SER
1	A	354	HIS
1	A	369	ASP
1	A	386	LYS
1	A	388	THR
1	A	390	GLU
1	A	395	LEU
1	A	412	GLU
1	A	422	LEU
1	A	470	LYS
1	B	255	LEU
1	B	272	LYS
1	B	323	HIS
1	B	349	LYS
1	B	350	LEU
1	B	352	SER
1	B	354	HIS
1	B	368	SER
1	B	462	MET
1	B	470	LYS
1	B	478	ILE

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Mol	Chain	Res	Type
2	D	688	LEU
2	E	686	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	HIS
1	A	432	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	$\# Z > 2$
3	XD5	A	501	-	19,19,19	1.42	2 (10%)	25,27,27	1.40	3 (12%)
3	XD5	B	501	-	19,19,19	1.59	2 (10%)	25,27,27	1.80	3 (12%)

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	XD5	A	501	-	-	0/8/25/25	0/4/3/3
3	XD5	B	501	-	-	0/8/25/25	0/4/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	XD5	O-C6	4.66	1.44	1.34
3	A	501	XD5	O-C6	4.58	1.43	1.34
3	B	501	XD5	O-C7	-2.75	1.41	1.46
3	A	501	XD5	O-C7	-2.72	1.41	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	XD5	O-C6-C4	6.89	123.05	111.92
3	A	501	XD5	O-C6-C4	4.90	119.84	111.92
3	B	501	XD5	C12-C7-C8	-3.13	100.15	104.34
3	A	501	XD5	C7-O-C6	-2.38	113.25	117.38
3	A	501	XD5	O-C6-O1	-2.22	119.91	123.53
3	B	501	XD5	O-C6-O1	-2.11	120.08	123.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/227 (98%)	-0.08	1 (0%) 92 91	24, 45, 77, 93	0
1	B	227/227 (100%)	-0.17	3 (1%) 77 75	16, 36, 64, 85	0
2	D	11/11 (100%)	-0.42	0 100 100	27, 34, 53, 71	0
2	E	10/11 (90%)	-0.40	0 100 100	19, 26, 35, 40	0
All	All	472/476 (99%)	-0.14	4 (0%) 86 84	16, 40, 72, 93	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	470	LYS	4.2
1	B	350	LEU	4.1
1	B	468	ASP	2.7
1	B	353	GLY	2.1

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. 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(\AA^2)	Q<0.9
3	XD5	A	501	17/17	-	-	40,44,46,47	17
3	XD5	B	501	17/17	-	-	34,39,47,48	17

6.5 Other polymers [i](#)

There are no such residues in this entry.