



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:31 PM UTC

PDB ID : 3II6 / pdb_00003ii6
Title : Structure of human Xrcc4 in complex with the tandem BRCT domains of DNA LigaseIV.
Authors : Meesala, S.; Junop, M.
Deposited on : 2009-07-31
Resolution : 2.40 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

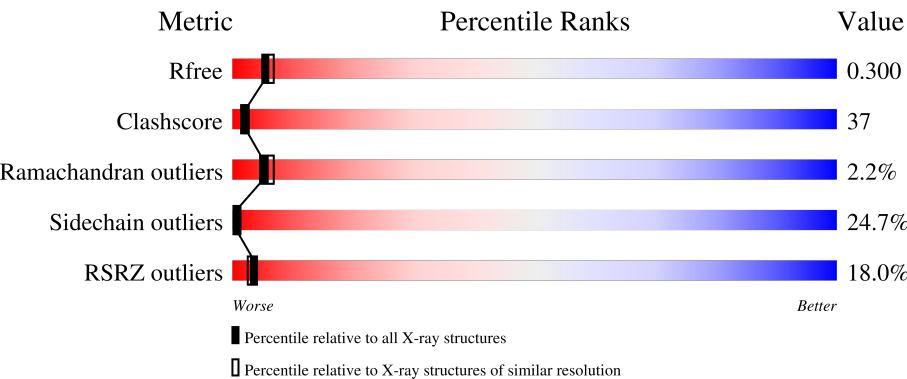
1 Overall quality at a glance i

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	203	20% 32% 44% 16% 7% .
1	B	203	33% 21% 48% 20% 7% .
1	C	203	20% 35% 36% 22% 5% .
1	D	203	35% 23% 44% 19% 9% .
2	X	263	3% 21% 33% 28% 15% .

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Mol	Chain	Length	Quality of chain
2	Y	263	3% 23% 41% 24% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10925 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 DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1631	1031	278	315	7			
1	B	196	Total	C	N	O	S	0	0	0
			1606	1016	273	310	7			
1	C	201	Total	C	N	O	S	0	0	0
			1631	1031	278	315	7			
1	D	195	Total	C	N	O	S	0	0	0
			1598	1012	272	307	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLU	ALA	engineered mutation	UNP Q13426
A	134	THR	ILE	engineered mutation	UNP Q13426
B	60	GLU	ALA	engineered mutation	UNP Q13426
B	134	THR	ILE	engineered mutation	UNP Q13426
C	60	GLU	ALA	engineered mutation	UNP Q13426
C	134	THR	ILE	engineered mutation	UNP Q13426
D	60	GLU	ALA	engineered mutation	UNP Q13426
D	134	THR	ILE	engineered mutation	UNP Q13426

- Molecule 2 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	256	Total	C	N	O	S	0	0	0
			2081	1326	351	391	13			
2	Y	258	Total	C	N	O	S	0	0	0
			2095	1333	353	396	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	649	GLY	-	expression tag	UNP P49917
X	650	ALA	-	expression tag	UNP P49917
X	651	MET	-	expression tag	UNP P49917
X	652	GLY	-	expression tag	UNP P49917
X	653	SER	-	expression tag	UNP P49917
Y	649	GLY	-	expression tag	UNP P49917
Y	650	ALA	-	expression tag	UNP P49917
Y	651	MET	-	expression tag	UNP P49917
Y	652	GLY	-	expression tag	UNP P49917
Y	653	SER	-	expression tag	UNP P49917

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Y	2	Total Cl 2 2	0	0

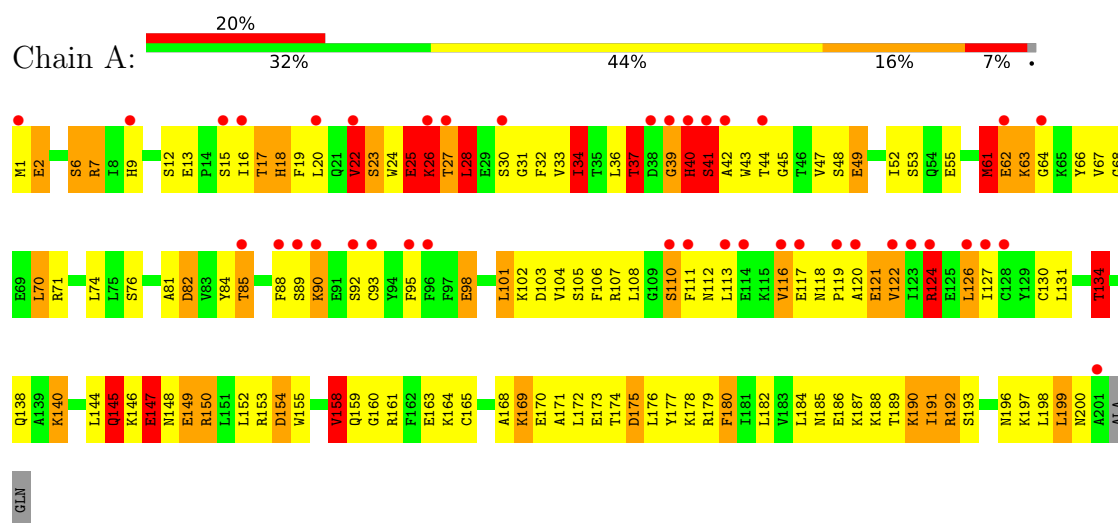
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0
4	B	25	Total O 25 25	0	0
4	C	41	Total O 41 41	0	0
4	D	29	Total O 29 29	0	0
4	X	83	Total O 83 83	0	0
4	Y	59	Total O 59 59	0	0

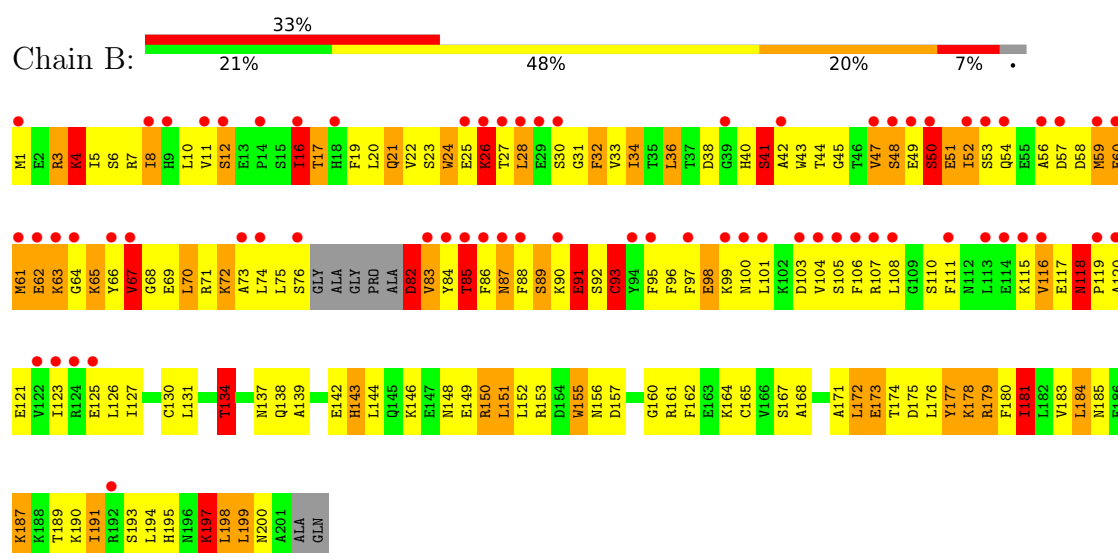
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: DNA repair protein XRCC4

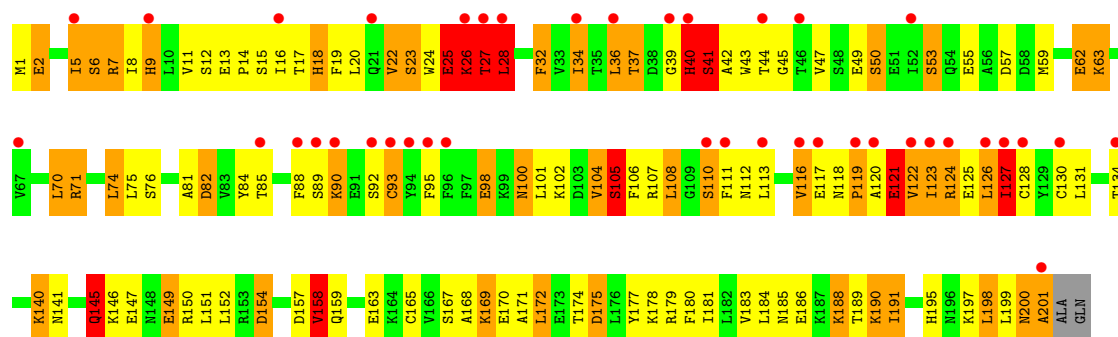


• Molecule 1: DNA repair protein XRCC4

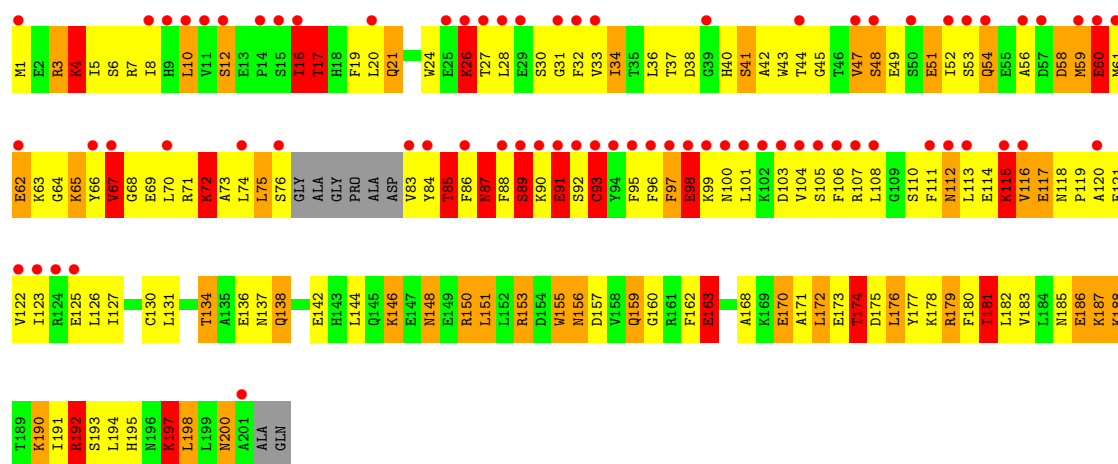


• Molecule 1: DNA repair protein XRCC4

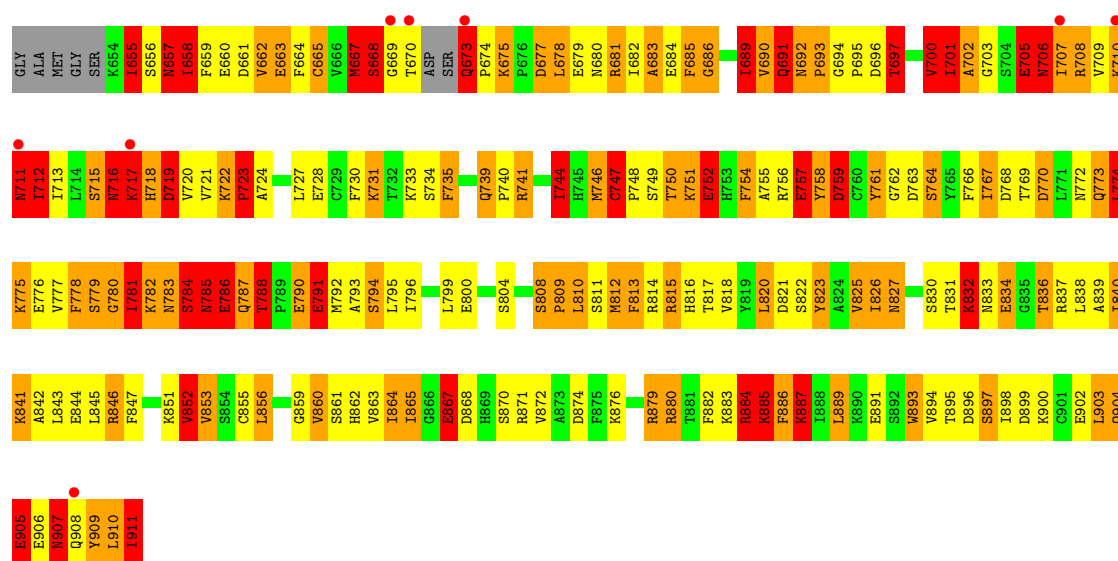
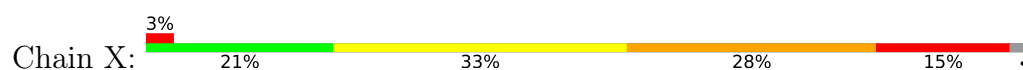




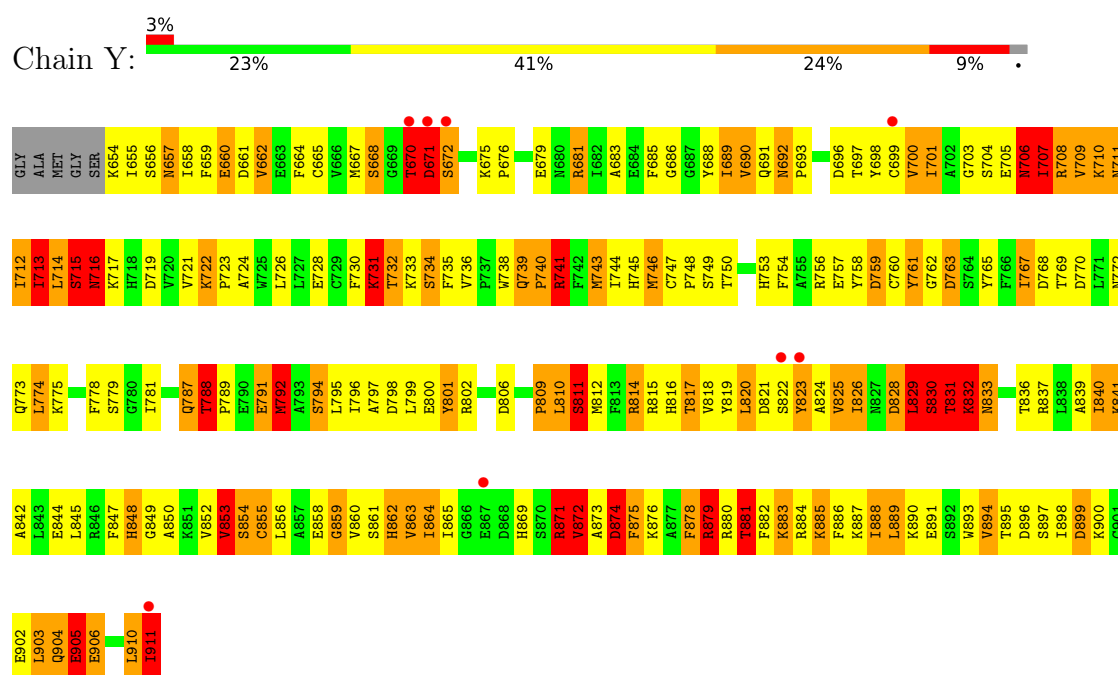
- Molecule 1: DNA repair protein XRCC4



- Molecule 2: DNA ligase 4



- Molecule 2: DNA ligase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.24Å 85.98Å 111.61Å 67.34° 82.86° 74.52°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.9 (20.00-2.40) 96.4 (20.00-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.280 0.254 , 0.300	Depositor DCC
R_{free} test set	3599 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10925	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: CL

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	2.24	72/1660 (4.3%)	1.91	56/2232 (2.5%)
1	B	2.00	51/1633 (3.1%)	1.75	41/2193 (1.9%)
1	C	2.17	68/1660 (4.1%)	1.86	46/2232 (2.1%)
1	D	2.00	43/1625 (2.6%)	1.92	58/2182 (2.7%)
2	X	2.69	160/2129 (7.5%)	2.37	135/2873 (4.7%)
2	Y	2.47	122/2144 (5.7%)	2.22	87/2895 (3.0%)
All	All	2.30	516/10851 (4.8%)	2.04	423/14607 (2.9%)

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	3
1	B	0	2
1	C	0	3
1	D	0	1
2	X	1	14
2	Y	0	12
All	All	1	35

The worst 5 of 516 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	52	ILE	C-O	15.91	1.44	1.24
2	X	781	ILE	CA-C	15.76	1.72	1.52
2	X	781	ILE	CA-CB	13.89	1.73	1.54
1	A	9	HIS	CE1-NE2	13.43	1.46	1.32
2	Y	818	VAL	CA-CB	13.20	1.72	1.54

The worst 5 of 423 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	722	LYS	CA-C-N	14.65	136.47	119.47
2	Y	722	LYS	C-N-CA	14.65	136.47	119.47
2	X	782	LYS	N-CA-C	13.23	129.73	110.42
2	X	785	ASN	N-CA-C	-13.15	94.65	114.64
2	X	904	GLN	N-CA-C	-12.78	94.69	110.41

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	X	911	ILE	CA

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	GLU	Peptide
1	A	26	LYS	Peptide
1	A	39	GLY	Peptide
1	B	82	ASP	Peptide
1	B	83	VAL	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	1631	0	1617	90	0
1	B	1606	0	1593	151	0
1	C	1631	0	1617	98	0
1	D	1598	0	1589	144	0
2	X	2081	0	2036	198	0
2	Y	2095	0	2046	151	0
3	Y	2	0	0	0	0
4	A	44	0	0	2	0
4	B	25	0	0	2	0
4	C	41	0	0	4	0
4	D	29	0	0	5	0
4	X	83	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Y	59	0	0	3	0
All	All	10925	0	10498	780	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 37.

The worst 5 of 780 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)
2:X:846:ARG:CD	2:X:846:ARG:CG	1.75	1.61
1:B:82:ASP:N	1:B:83:VAL:HG23	1.09	1.36
1:A:127:ILE:HD11	1:B:127:ILE:CD1	1.65	1.27
1:B:82:ASP:N	1:B:83:VAL:CG2	1.95	1.26
1:C:40:HIS:CD2	1:D:120:ALA:HB2	1.73	1.22

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	199/203 (98%)	170 (85%)	26 (13%)	3 (2%)	8	12
1	B	192/203 (95%)	168 (88%)	19 (10%)	5 (3%)	4	4
1	C	199/203 (98%)	172 (86%)	22 (11%)	5 (2%)	4	5
1	D	191/203 (94%)	167 (87%)	19 (10%)	5 (3%)	4	4
2	X	252/263 (96%)	217 (86%)	32 (13%)	3 (1%)	10	16
2	Y	256/263 (97%)	221 (86%)	27 (10%)	8 (3%)	3	3
All	All	1289/1338 (96%)	1115 (86%)	145 (11%)	29 (2%)	5	6

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	50	SER
2	X	747	CYS
2	X	786	GLU
2	Y	829	LEU
1	A	34	ILE

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	181/182 (100%)	137 (76%)	44 (24%)	1	1
1	B	180/182 (99%)	130 (72%)	50 (28%)	0	0
1	C	181/182 (100%)	141 (78%)	40 (22%)	1	1
1	D	179/182 (98%)	132 (74%)	47 (26%)	0	0
2	X	232/236 (98%)	170 (73%)	62 (27%)	0	0
2	Y	234/236 (99%)	184 (79%)	50 (21%)	1	1
All	All	1187/1200 (99%)	894 (75%)	293 (25%)	1	1

5 of 293 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	852	VAL
2	Y	879	ARG
2	X	884	ARG
2	Y	740	PRO
1	C	12	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	X	816	HIS
2	Y	848	HIS
2	X	848	HIS
2	Y	745	HIS

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Mol	Chain	Res	Type
2	Y	907	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [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 [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(Å²)	Q<0.9
1	A	201/203 (99%)	0.92	40 (19%)	3	2	35, 71, 104, 125	0
1	B	196/203 (96%)	1.48	67 (34%)	1	1	33, 99, 134, 147	0
1	C	201/203 (99%)	0.99	40 (19%)	3	2	32, 72, 103, 132	0
1	D	195/203 (96%)	1.60	72 (36%)	1	0	29, 94, 134, 148	0
2	X	256/263 (97%)	0.16	8 (3%)	51	47	31, 50, 83, 96	0
2	Y	258/263 (98%)	0.18	8 (3%)	51	47	33, 49, 79, 112	0
All	All	1307/1338 (97%)	0.82	235 (17%)	3	3	29, 63, 125, 148	0

The worst 5 of 235 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	56	ALA	6.9
1	D	59	MET	6.5
1	B	61	MET	5.9
1	D	61	MET	5.9
1	A	39	GLY	5.6

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 oligosaccharides 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
3	CL	Y	302	1/1	0.92	0.10	65,65,65,65	0
3	CL	Y	301	1/1	0.94	0.10	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.