



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:28 AM GMT

PDB ID : 3LW0  
Title : IGF-1RK in complex with ligand MSC1609119A-1  
Authors : Graedler, U.; Heinrich, T.; Boettcher, H.; Blaukat, A.; Shutes, A.; Askew, B.  
Deposited on : 2010-02-23  
Resolution : 1.79 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.

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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

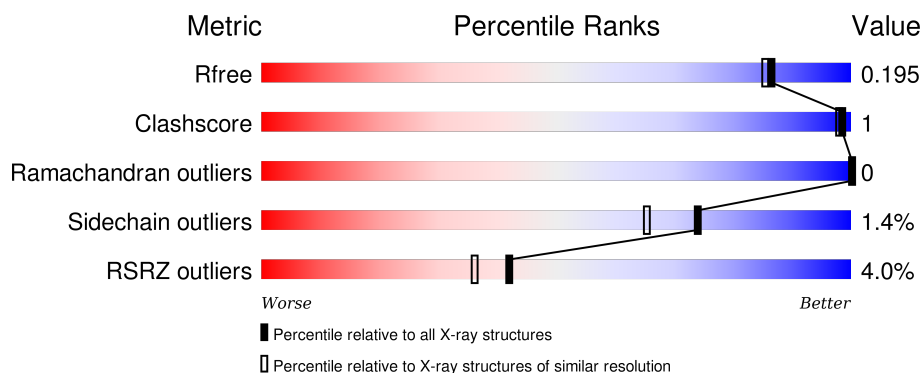
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	304	<div> <div>4%</div> <div>92%</div> <div>• •</div> </div>
1	B	304	<div> <div>4%</div> <div>93%</div> <div>• •</div> </div>
1	C	304	<div> <div>4%</div> <div>93%</div> <div>• • •</div> </div>
1	D	304	<div> <div>4%</div> <div>92%</div> <div>• •</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CCX	A	1	-	-	-	X
2	CCX	B	2	-	-	-	X
2	CCX	C	3	-	-	-	X
2	CCX	D	4	-	-	-	X
3	GOL	C	2	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10929 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.

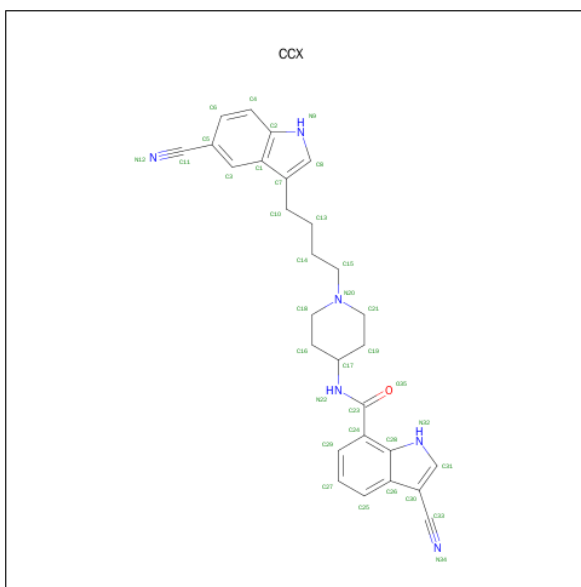
- Molecule 1 is a protein called Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	23	6	0
			2392	1518	398	451	25			
1	B	292	Total	C	N	O	S	10	8	0
			2407	1526	401	455	25			
1	C	292	Total	C	N	O	S	12	6	0
			2392	1518	398	451	25			
1	D	292	Total	C	N	O	S	21	6	0
			2393	1519	398	451	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1097	ALA	GLU	ENGINEERED MUTATION	UNP P08069
A	1099	ALA	GLU	ENGINEERED MUTATION	UNP P08069
B	1097	ALA	GLU	ENGINEERED MUTATION	UNP P08069
B	1099	ALA	GLU	ENGINEERED MUTATION	UNP P08069
C	1097	ALA	GLU	ENGINEERED MUTATION	UNP P08069
C	1099	ALA	GLU	ENGINEERED MUTATION	UNP P08069
D	1097	ALA	GLU	ENGINEERED MUTATION	UNP P08069
D	1099	ALA	GLU	ENGINEERED MUTATION	UNP P08069

- Molecule 2 is 3-CYANO-N-{1-[4-(5-CYANO-1H-INDOL-3-YL)BUTYL]PIPERIDIN-4-YL}-1H-INDOLE-7-CARBOXAMIDE (three-letter code: CCX) (formula: C<sub>28</sub>H<sub>28</sub>N<sub>6</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	13	0
			35	28	6	1		
2	A	1	Total	C	N	O	0	0
			35	28	6	1		
2	B	1	Total	C	N	O	13	0
			35	28	6	1		
2	B	1	Total	C	N	O	0	0
			35	28	6	1		
2	C	1	Total	C	N	O	14	0
			35	28	6	1		
2	C	1	Total	C	N	O	0	0
			35	28	6	1		
2	D	1	Total	C	N	O	13	0
			35	28	6	1		
2	D	1	Total	C	N	O	0	0
			35	28	6	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

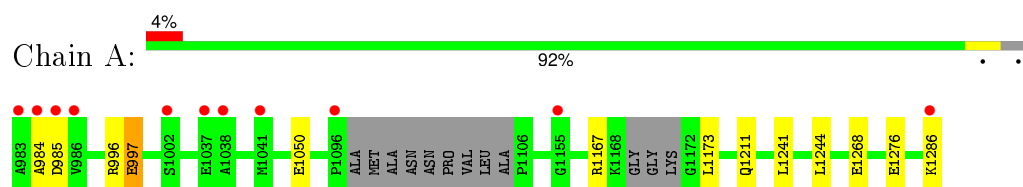
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	279	Total	O	0	1
			280	280		
4	B	254	Total	O	0	1
			255	255		
4	C	263	Total	O	0	1
			264	264		
4	D	253	Total	O	0	1
			254	254		

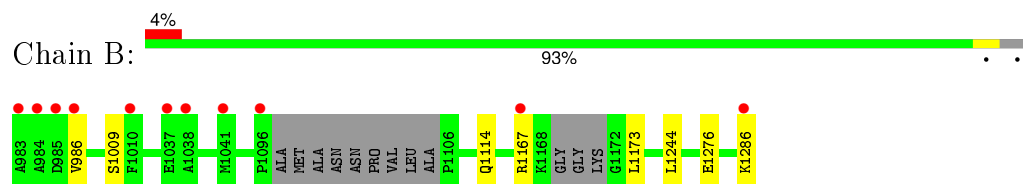
### 3 Residue-property plots [i](#)

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.

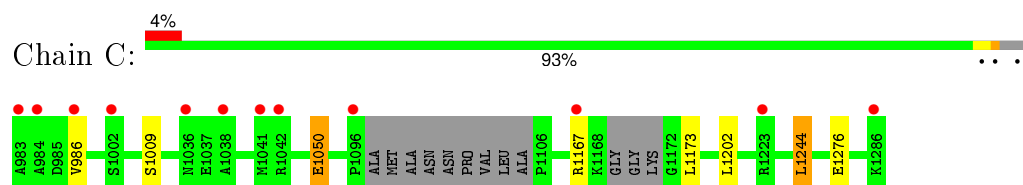
- Molecule 1: Insulin-like growth factor 1 receptor



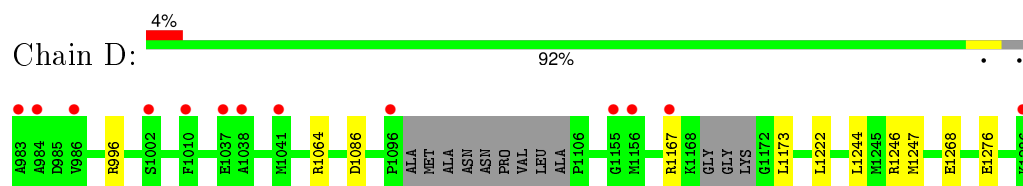
- Molecule 1: Insulin-like growth factor 1 receptor



- Molecule 1: Insulin-like growth factor 1 receptor



- Molecule 1: Insulin-like growth factor 1 receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.35Å 189.35Å 115.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.79 94.66 – 1.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.79) 99.8 (94.66-1.79)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.157 , 0.185 0.169 , 0.195	Depositor DCC
$R_{free}$ test set	4952 reflections (3.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.5	EDS
Estimated twinning fraction	0.025 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.025 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.025 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.467 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.470 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.467 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.026 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 145764 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10929	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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

### 5.1 Standard geometry

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

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	0.55	1/2441 (0.0%)	0.64	0/3287
1	B	0.53	0/2456	0.61	0/3308
1	C	0.55	1/2441 (0.0%)	0.63	0/3287
1	D	0.53	0/2442	0.62	0/3289
All	All	0.54	2/9780 (0.0%)	0.63	0/13171

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1050	GLU	CG-CD	6.98	1.62	1.51
1	A	1050	GLU	CG-CD	6.29	1.61	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1050	GLU	Sidechain

## 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	2392	0	2346	6	0
1	B	2407	0	2358	5	0
1	C	2392	0	2346	4	0
1	D	2393	0	2349	5	0
2	A	70	0	56	0	0
2	B	70	0	56	0	0
2	C	70	0	56	0	0
2	D	70	0	56	0	0
3	B	6	0	8	1	0
3	C	6	0	8	0	0
4	A	280	0	0	1	0
4	B	255	0	0	1	0
4	C	264	0	0	1	0
4	D	254	0	0	3	0
All	All	10929	0	9639	18	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 1.

All (18) 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:A:1276[A]:GLU:OE2	1:D:1276[A]:GLU:OE2	2.05	0.74
1:D:1247[B]:MET:SD	4:D:773:HOH:O	2.56	0.62
1:B:1276[A]:GLU:OE2	1:C:1276[A]:GLU:OE2	2.24	0.56
1:A:997:GLU:CD	1:A:997:GLU:H	2.08	0.55
1:B:1114:GLN:HG3	3:B:1:GOL:H12	1.89	0.55
1:D:1167:ARG:HB2	1:D:1173:LEU:HD23	1.91	0.52
1:D:1246:ARG:NH1	4:D:685:HOH:O	2.42	0.51
1:B:1286:LYS:OXT	1:B:1286:LYS:HG3	2.12	0.50
1:C:1009:SER:HB3	4:C:1301:HOH:O	2.12	0.49
1:A:1286:LYS:HG3	1:A:1286:LYS:OXT	2.13	0.49
1:B:1009:SER:HB3	4:B:781:HOH:O	2.13	0.49
1:D:1064:ARG:HD2	4:D:897:HOH:O	2.13	0.48
1:C:1167:ARG:HB2	1:C:1173:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1167:ARG:HB2	1:B:1173:LEU:HD23	1.98	0.45
1:A:1211:GLN:HG3	4:A:388:HOH:O	2.15	0.45
1:A:984:ALA:O	1:A:985:ASP:HB2	2.17	0.45
1:A:1167:ARG:HB2	1:A:1173:LEU:HD23	2.00	0.43
1:C:1202:LEU:HD11	1:C:1244:LEU:HD13	2.00	0.43

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	292/304 (96%)	286 (98%)	6 (2%)	0	100	100
1	B	294/304 (97%)	288 (98%)	6 (2%)	0	100	100
1	C	292/304 (96%)	285 (98%)	7 (2%)	0	100	100
1	D	292/304 (96%)	286 (98%)	6 (2%)	0	100	100
All	All	1170/1216 (96%)	1145 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	262/263 (100%)	257 (98%)	5 (2%)	65	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	264/263 (100%)	262 (99%)	2 (1%)	86	83
1	C	262/263 (100%)	260 (99%)	2 (1%)	86	83
1	D	262/263 (100%)	257 (98%)	5 (2%)	65	52
All	All	1050/1052 (100%)	1036 (99%)	14 (1%)	74	68

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	996	ARG
1	A	997	GLU
1	A	1241	LEU
1	A	1244	LEU
1	A	1268	GLU
1	B	986	VAL
1	B	1244	LEU
1	C	986	VAL
1	C	1244	LEU
1	D	996	ARG
1	D	1086	ASP
1	D	1222	LEU
1	D	1244	LEU
1	D	1268	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1214	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 ⓘ

10 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	CCX	A	1	-	36,39,39	1.36	3 (8%)	41,54,54	1.43	9 (21%)
2	CCX	A	1287	-	36,39,39	1.17	3 (8%)	41,54,54	1.23	4 (9%)
3	GOL	B	1	-	5,5,5	0.35	0	5,5,5	0.50	0
2	CCX	B	1287	-	36,39,39	1.19	3 (8%)	41,54,54	1.33	7 (17%)
2	CCX	B	2	-	36,39,39	1.31	4 (11%)	41,54,54	1.32	7 (17%)
2	CCX	C	1287	-	36,39,39	1.14	3 (8%)	41,54,54	1.28	4 (9%)
3	GOL	C	2	-	5,5,5	0.37	0	5,5,5	0.45	0
2	CCX	C	3	-	36,39,39	1.40	4 (11%)	41,54,54	1.45	8 (19%)
2	CCX	D	1287	-	36,39,39	1.26	4 (11%)	41,54,54	1.30	8 (19%)
2	CCX	D	4	-	36,39,39	1.14	2 (5%)	41,54,54	1.99	9 (21%)

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	CCX	A	1	-	-	0/17/29/29	0/5/5/5
2	CCX	A	1287	-	-	0/17/29/29	0/5/5/5
3	GOL	B	1	-	-	0/4/4/4	0/0/0/0
2	CCX	B	1287	-	-	0/17/29/29	0/5/5/5
2	CCX	B	2	-	-	0/17/29/29	0/5/5/5
2	CCX	C	1287	-	-	0/17/29/29	0/5/5/5
3	GOL	C	2	-	-	0/4/4/4	0/0/0/0
2	CCX	C	3	-	-	0/17/29/29	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CCX	D	1287	-	-	0/17/29/29	0/5/5/5
2	CCX	D	4	-	-	0/17/29/29	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	CCX	C30-C26	-3.49	1.37	1.42
2	D	4	CCX	C30-C26	-3.27	1.37	1.42
2	B	2	CCX	C30-C26	-3.10	1.38	1.42
2	C	3	CCX	C30-C26	-3.07	1.38	1.42
2	D	1287	CCX	C30-C26	-2.67	1.38	1.42
2	B	1287	CCX	C30-C26	-2.50	1.38	1.42
2	C	3	CCX	C24-C28	-2.48	1.39	1.43
2	D	1287	CCX	C24-C28	-2.44	1.39	1.43
2	B	2	CCX	C24-C28	-2.43	1.39	1.43
2	A	1	CCX	C24-C28	-2.42	1.39	1.43
2	D	4	CCX	C24-C28	-2.38	1.39	1.43
2	C	1287	CCX	C30-C26	-2.24	1.39	1.42
2	C	1287	CCX	C3-C1	-2.20	1.38	1.42
2	A	1287	CCX	C25-C26	-2.16	1.37	1.42
2	B	1287	CCX	C24-C23	-2.16	1.47	1.50
2	A	1287	CCX	C30-C26	-2.13	1.39	1.42
2	D	1287	CCX	C3-C1	-2.12	1.38	1.42
2	B	2	CCX	C4-C6	2.00	1.40	1.36
2	C	1287	CCX	C23-N22	2.03	1.38	1.34
2	C	3	CCX	C23-N22	2.08	1.38	1.34
2	B	1287	CCX	C23-N22	2.14	1.39	1.34
2	D	1287	CCX	C23-N22	2.15	1.39	1.34
2	A	1287	CCX	C23-N22	2.23	1.39	1.34
2	B	2	CCX	C23-N22	3.92	1.43	1.34
2	A	1	CCX	C23-N22	4.30	1.43	1.34
2	C	3	CCX	C33-N34	4.65	1.25	1.14

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	CCX	C30-C33-N34	-4.22	164.11	176.54
2	A	1287	CCX	C19-C17-N22	-3.81	103.50	110.56
2	B	1287	CCX	C19-C17-N22	-3.65	103.80	110.56
2	D	1287	CCX	C19-C17-N22	-3.55	103.98	110.56
2	A	1	CCX	C5-C3-C1	-3.44	117.48	121.50
2	C	1287	CCX	C19-C17-N22	-3.43	104.21	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	CCX	C25-C26-C30	-3.23	130.01	135.57
2	B	2	CCX	C5-C3-C1	-3.11	117.88	121.50
2	D	4	CCX	C5-C3-C1	-3.09	117.89	121.50
2	D	4	CCX	C25-C26-C30	-3.07	130.29	135.57
2	C	3	CCX	C5-C3-C1	-2.98	118.03	121.50
2	C	1287	CCX	C5-C3-C1	-2.83	118.21	121.50
2	B	2	CCX	C25-C26-C30	-2.74	130.85	135.57
2	C	3	CCX	C25-C26-C30	-2.71	130.90	135.57
2	B	1287	CCX	C25-C26-C30	-2.63	131.05	135.57
2	A	1287	CCX	C25-C26-C30	-2.54	131.19	135.57
2	B	1287	CCX	C5-C3-C1	-2.54	118.54	121.50
2	A	1	CCX	C6-C4-C2	-2.49	118.18	120.88
2	D	1287	CCX	C25-C26-C30	-2.45	131.35	135.57
2	A	1287	CCX	C5-C3-C1	-2.42	118.68	121.50
2	C	1287	CCX	C25-C26-C30	-2.36	131.50	135.57
2	B	2	CCX	C6-C4-C2	-2.34	118.34	120.88
2	D	1287	CCX	O35-C23-C24	-2.32	118.18	121.59
2	A	1	CCX	C19-C17-C16	-2.27	106.96	110.82
2	D	4	CCX	C6-C4-C2	-2.16	118.53	120.88
2	A	1	CCX	C18-C16-C17	-2.14	106.94	110.37
2	B	2	CCX	O35-C23-C24	-2.13	118.45	121.59
2	C	3	CCX	C6-C4-C2	-2.09	118.61	120.88
2	D	1287	CCX	C5-C3-C1	-2.04	119.12	121.50
2	D	4	CCX	O35-C23-N22	-2.03	118.78	122.44
2	A	1	CCX	C27-C25-C26	-2.01	118.04	120.88
2	D	4	CCX	C27-C25-C26	-2.01	118.05	120.88
2	D	1287	CCX	C24-C23-N22	2.00	120.59	116.86
2	B	2	CCX	C24-C23-N22	2.02	120.62	116.86
2	A	1	CCX	C21-N20-C18	2.02	113.27	108.90
2	A	1287	CCX	C25-C26-C28	2.04	121.25	117.03
2	B	1287	CCX	C24-C23-N22	2.05	120.67	116.86
2	B	1287	CCX	C3-C1-C2	2.05	121.15	120.34
2	C	1287	CCX	C3-C1-C2	2.06	121.16	120.34
2	D	1287	CCX	C25-C26-C28	2.08	121.33	117.03
2	D	1287	CCX	C3-C5-C11	2.12	121.56	119.63
2	C	3	CCX	C25-C26-C28	2.15	121.47	117.03
2	C	3	CCX	C24-C23-N22	2.16	120.88	116.86
2	B	1287	CCX	C25-C26-C28	2.20	121.57	117.03
2	B	2	CCX	C25-C26-C28	2.20	121.58	117.03
2	D	1287	CCX	C17-N22-C23	2.24	125.32	122.52
2	D	4	CCX	C25-C26-C28	2.33	121.84	117.03
2	C	3	CCX	C17-N22-C23	2.45	125.58	122.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	CCX	C25-C26-C28	2.47	122.12	117.03
2	D	4	CCX	C24-C23-N22	2.54	121.59	116.86
2	B	1287	CCX	C21-C19-C17	2.73	114.77	110.37
2	C	3	CCX	C3-C1-C2	2.98	121.52	120.34
2	A	1	CCX	C3-C1-C2	3.43	121.70	120.34
2	B	2	CCX	C3-C1-C2	4.02	121.93	120.34
2	D	4	CCX	C3-C1-C2	4.25	122.02	120.34
2	D	4	CCX	C17-N22-C23	8.96	133.70	122.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	GOL	1	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, 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	292/304 (96%)	0.24	11 (3%) 44 38	4, 12, 23, 35	15 (5%)
1	B	292/304 (96%)	0.25	11 (3%) 44 38	3, 12, 23, 35	9 (3%)
1	C	292/304 (96%)	0.25	12 (4%) 41 35	4, 12, 23, 34	7 (2%)
1	D	292/304 (96%)	0.23	13 (4%) 37 31	4, 12, 24, 34	15 (5%)
All	All	1168/1216 (96%)	0.24	47 (4%) 42 36	3, 12, 24, 35	46 (3%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	983	ALA	6.7
1	C	984	ALA	6.2
1	B	984	ALA	5.6
1	D	984	ALA	5.2
1	D	1096	PRO	4.6
1	A	1096	PRO	4.4
1	D	983	ALA	4.4
1	C	1038	ALA	3.7
1	D	1286	LYS	3.7
1	B	1286	LYS	3.7
1	B	983	ALA	3.7
1	A	1041	MET	3.3
1	A	1286	LYS	3.3
1	C	1096	PRO	3.2
1	B	985	ASP	3.1
1	A	1038	ALA	3.1
1	C	1286	LYS	3.1
1	B	1038	ALA	3.1
1	C	1042	ARG	3.1
1	B	1096	PRO	3.1
1	C	1041	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	1038	ALA	3.0
1	B	1041	MET	2.9
1	D	1167	ARG	2.8
1	C	986	VAL	2.8
1	C	1167	ARG	2.8
1	B	986	VAL	2.7
1	C	983	ALA	2.7
1	A	984	ALA	2.5
1	A	985	ASP	2.4
1	A	1002	SER	2.3
1	D	1155	GLY	2.3
1	C	1036	ASN	2.3
1	B	1167	ARG	2.3
1	D	1156	MET	2.2
1	C	1002	SER	2.2
1	D	986	VAL	2.2
1	A	1037	GLU	2.2
1	B	1010	PHE	2.1
1	D	1041	MET	2.1
1	D	1002	SER	2.1
1	C	1223	ARG	2.1
1	A	1155	GLY	2.1
1	D	1037	GLU	2.0
1	B	1037	GLU	2.0
1	A	986	VAL	2.0
1	D	1010	PHE	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( $\text{\AA}^2$ )	Q<0.9
2	CCX	A	1	35/35	0.90	0.22	5.85	12,23,31,34	13
2	CCX	C	3	35/35	0.91	0.22	5.77	14,22,24,24	14
2	CCX	D	4	35/35	0.91	0.22	3.97	13,22,32,35	13
2	CCX	B	2	35/35	0.91	0.21	3.69	13,23,30,32	13
3	GOL	C	2	6/6	0.84	0.27	3.24	42,44,45,48	0
2	CCX	B	1287	35/35	0.96	0.08	-1.21	4,10,15,18	0
2	CCX	C	1287	35/35	0.96	0.08	-1.30	5,10,15,17	0
2	CCX	A	1287	35/35	0.96	0.08	-1.49	4,10,15,18	0
2	CCX	D	1287	35/35	0.96	0.08	-1.49	3,9,14,18	0
3	GOL	B	1	6/6	0.75	0.36	-	48,49,49,49	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.