



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:28 AM UTC

PDB ID : 2CKB / pdb\_00002ckb  
Title : STRUCTURE OF THE 2C/KB/DEV8 COMPLEX  
Authors : Garcia, K.C.; Degano, M.; Wilson, I.A.  
Deposited on : 1998-01-14  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

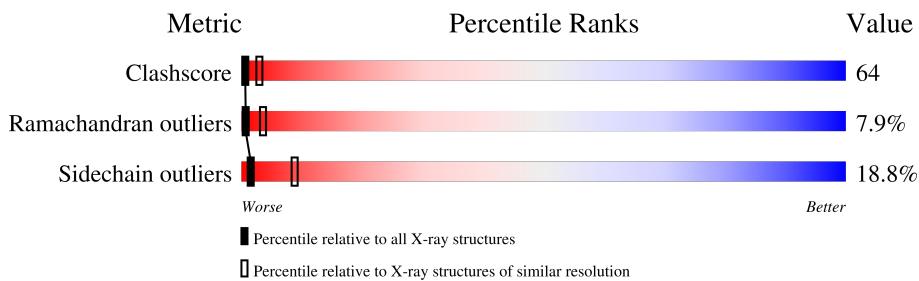
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

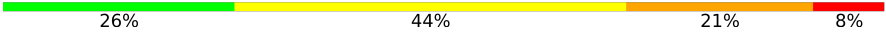
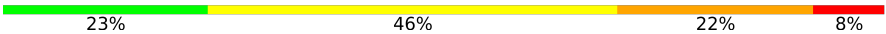
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	202	23% 56% 18% .
1	C	202	22% 56% 19% .
2	B	237	24% 55% 18% .
2	D	237	23% 56% 19% .
3	H	274	25% 60% 14% .
3	I	274	23% 61% 15% .
4	P	8	25% 38% 38%
4	Q	8	25% 38% 38%

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Mol	Chain	Length	Quality of chain				
5	L	99		26%	44%	21%	8%
5	M	99		23%	46%	22%	8%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13110 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 ALPHA, BETA T CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	202	1570	999	253	310	8	0	0	0
1	C	202	1570	999	253	310	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	GLN	conflict	EMBL X01134
A	165	ALA	LYS	conflict	EMBL X01134
C	127	ALA	GLN	conflict	EMBL X01134
C	165	ALA	LYS	conflict	EMBL X01134

- Molecule 2 is a protein called ALPHA, BETA T CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	237	1853	1160	331	355	7	0	0	0
2	D	237	1853	1160	331	355	7	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	97	GLY	GLN	conflict	GB 1791255
B	?	-	ARG	deletion	GB 1791255
B	?	-	ALA	deletion	GB 1791255
B	105	THR	GLU	conflict	GB 1791255
B	106	LEU	GLN	conflict	GB 1791255
B	107	TYR	PHE	conflict	GB 1791255
B	110	ALA	PRO	conflict	GB 1791255
B	115	SER	THR	conflict	GB 1791255

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Chain	Residue	Modelled	Actual	Comment	Reference
D	97	GLY	GLN	conflict	GB 1791255
D	?	-	ARG	deletion	GB 1791255
D	?	-	ALA	deletion	GB 1791255
D	105	THR	GLU	conflict	GB 1791255
D	106	LEU	GLN	conflict	GB 1791255
D	107	TYR	PHE	conflict	GB 1791255
D	110	ALA	PRO	conflict	GB 1791255
D	115	SER	THR	conflict	GB 1791255

- Molecule 3 is a protein called MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I MOLECULE K(B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	274	Total	C	N	O	S	0	0	0
			2232	1408	393	422	9			
3	I	274	Total	C	N	O	S	0	0	0
			2232	1408	393	422	9			

- Molecule 4 is a protein called DEV8 PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	P	8	Total	C	N	O	0	0	0
			76	51	10	15			
4	Q	8	Total	C	N	O	0	0	0
			76	51	10	15			

- Molecule 5 is a protein called BETA-2 MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	L	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
5	M	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 6 is water.

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

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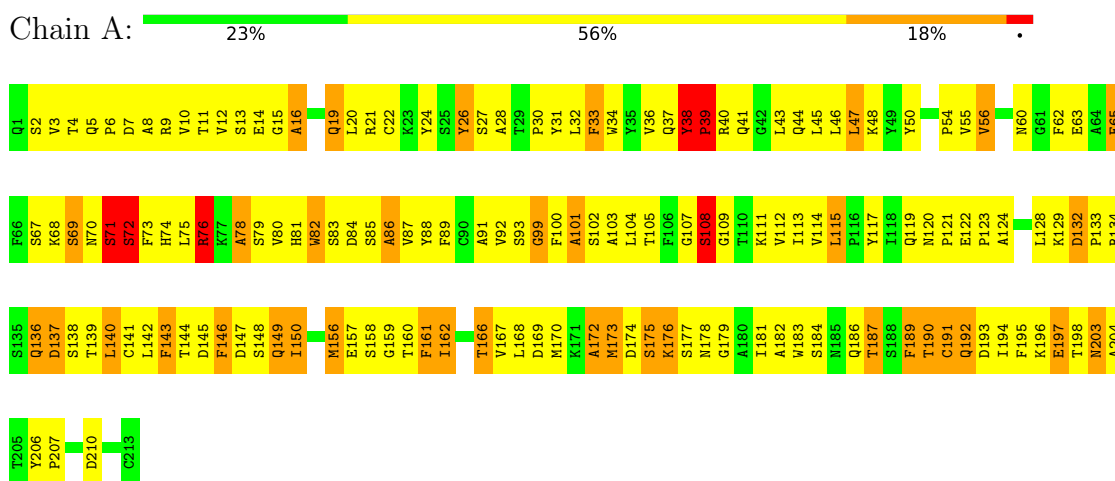
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total O 1 1	0	0
6	D	1	Total O 1 1	0	0
6	I	1	Total O 1 1	0	0
6	Q	1	Total O 1 1	0	0

### 3 Residue-property plots

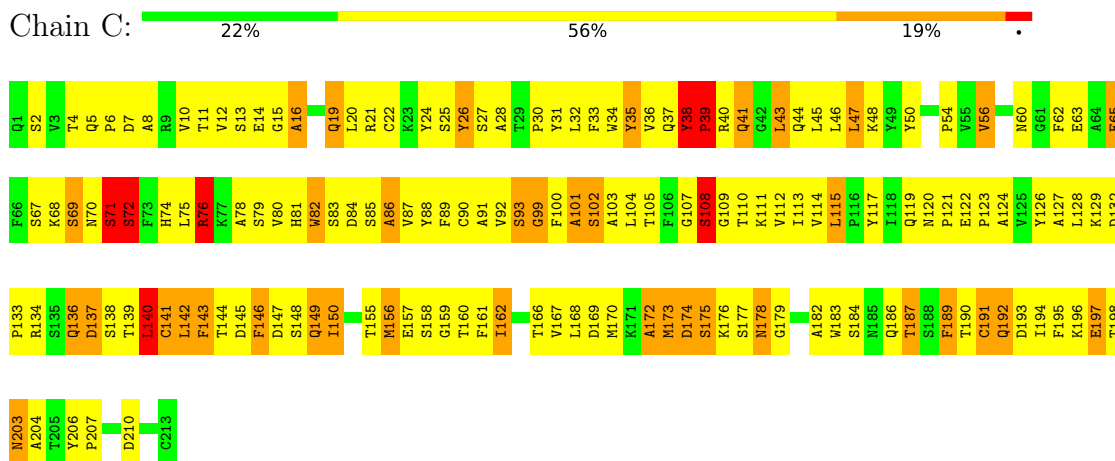
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: ALPHA, BETA T CELL RECEPTOR

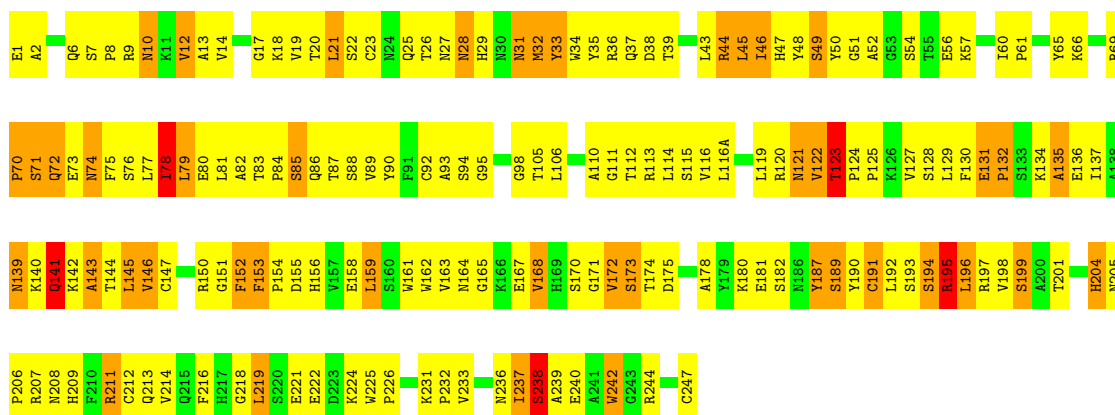


- Molecule 1: ALPHA, BETA T CELL RECEPTOR



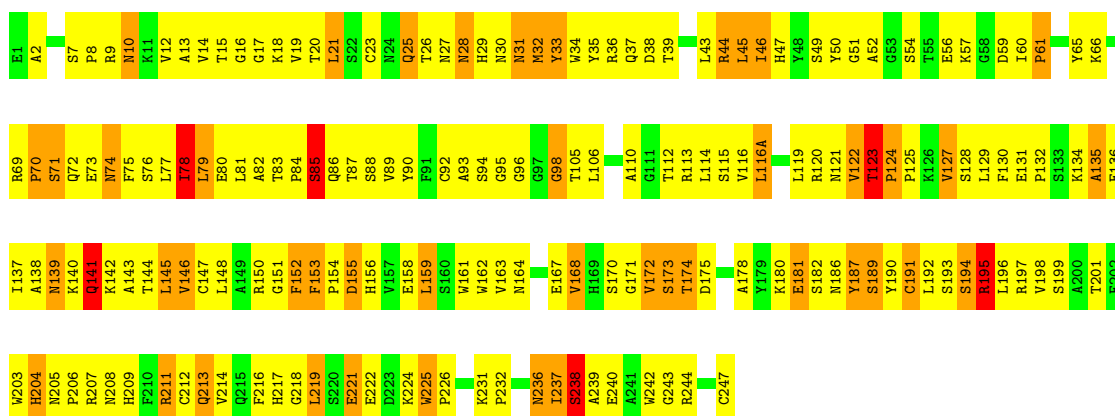
- Molecule 2: ALPHA, BETA T CELL RECEPTOR





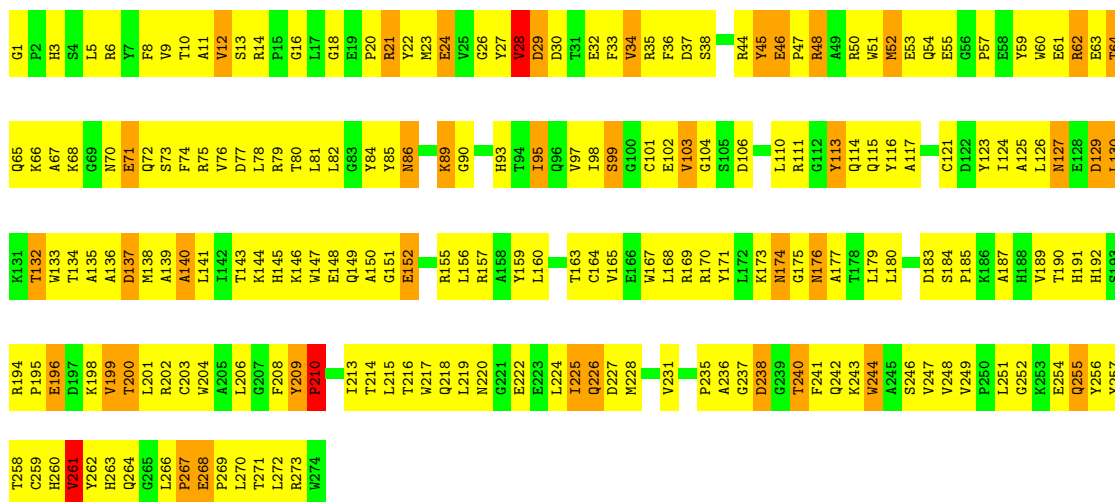
- Molecule 2: ALPHA, BETA T CELL RECEPTOR

Chain D: 23% 56% 19%

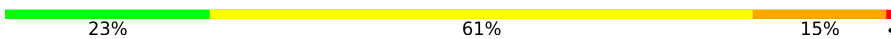


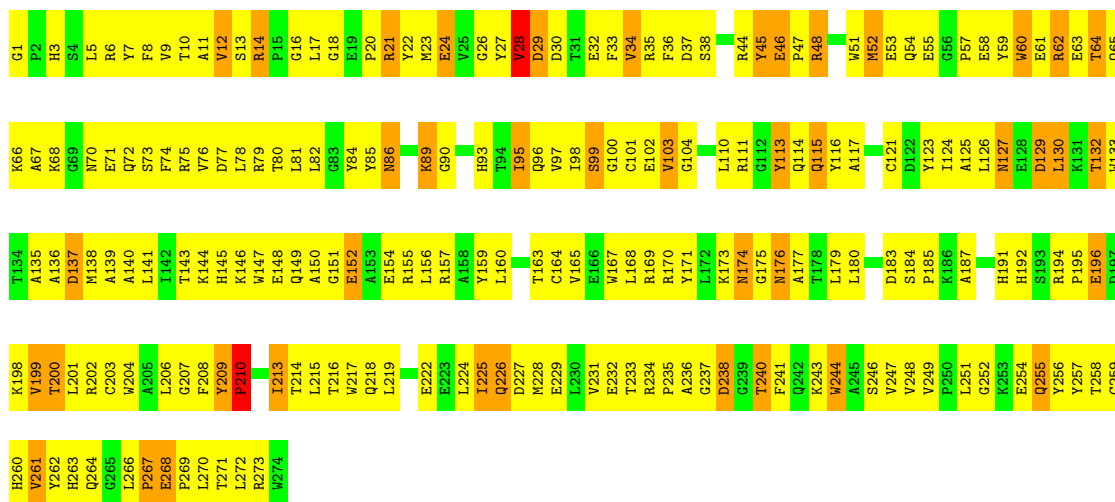
- Molecule 3: MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I MOLECULE K(B)

Chain H: 25% 60% 14%




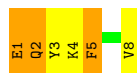
- Molecule 3: MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I MOLECULE K(B)

Chain I:  23% 61% 15%




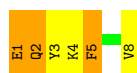
• Molecule 4: DEV8 PEPTIDE

Chain P:  25% 38% 38%

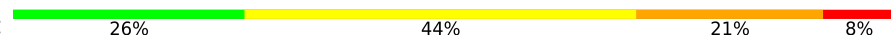


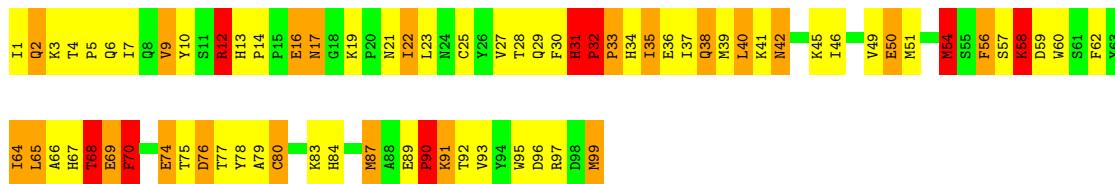
• Molecule 4: DEV8 PEPTIDE

Chain Q:  25% 38% 38%

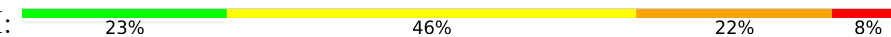


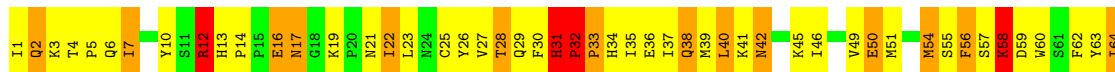
• Molecule 5: BETA-2 MICROGLOBULIN

Chain L:  26% 44% 21% 8%



• Molecule 5: BETA-2 MICROGLOBULIN

Chain M:  23% 46% 22% 8%





## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	295.66Å 89.96Å 84.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00	Depositor
% Data completeness (in resolution range)	78.7 (25.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.221 , 0.322	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13110	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

## 5 Model quality [i](#)

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

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	0.69	0/1611	1.24	18/2193 (0.8%)
1	C	0.67	0/1611	1.24	17/2193 (0.8%)
2	B	0.65	0/1904	1.20	22/2586 (0.9%)
2	D	0.72	0/1904	1.22	18/2586 (0.7%)
3	H	0.61	0/2293	1.03	8/3113 (0.3%)
3	I	0.60	0/2293	1.03	7/3113 (0.2%)
4	P	0.62	0/78	1.13	1/102 (1.0%)
4	Q	0.65	0/78	1.08	1/102 (1.0%)
5	L	0.64	0/847	1.32	13/1148 (1.1%)
5	M	0.62	0/847	1.32	13/1148 (1.1%)
All	All	0.65	0/13466	1.17	118/18284 (0.6%)

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
2	B	0	1
2	D	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	89	GLU	CA-C-N	11.05	133.65	119.84
5	M	89	GLU	C-N-CA	11.05	133.65	119.84
5	L	89	GLU	CA-C-N	11.04	133.63	119.84
5	L	89	GLU	C-N-CA	11.04	133.63	119.84
1	C	191	CYS	N-CA-C	-10.38	98.77	111.33

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	187	TYR	Sidechain
1	C	35	TYR	Sidechain
2	D	187	TYR	Sidechain

## 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	1570	0	1508	196	0
1	C	1570	0	1508	208	0
2	B	1853	0	1767	261	0
2	D	1853	0	1767	270	0
3	H	2232	0	2127	283	0
3	I	2232	0	2127	284	0
4	P	76	0	70	16	0
4	Q	76	0	70	19	0
5	L	821	0	798	104	0
5	M	821	0	798	108	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	2	0
6	H	1	0	0	1	0
6	I	1	0	0	1	0
6	Q	1	0	0	0	0
All	All	13110	0	12540	1628	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 64.

The worst 5 of 1628 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:B:153:PHE:CD1	2:B:154:PRO:HD3	1.82	1.14
1:A:146:PHE:HD2	1:A:150:ILE:HD11	1.03	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:138:MET:HA	3:H:141:LEU:HD12	1.31	1.13
3:H:215:LEU:HD21	3:H:261:VAL:HG13	1.33	1.10
2:D:181:GLU:HB3	2:D:189:SER:O	1.52	1.08

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	200/202 (99%)	144 (72%)	35 (18%)	21 (10%)	0	2
1	C	200/202 (99%)	146 (73%)	32 (16%)	22 (11%)	0	1
2	B	235/237 (99%)	181 (77%)	43 (18%)	11 (5%)	2	11
2	D	235/237 (99%)	181 (77%)	44 (19%)	10 (4%)	2	12
3	H	272/274 (99%)	205 (75%)	50 (18%)	17 (6%)	1	6
3	I	272/274 (99%)	203 (75%)	53 (20%)	16 (6%)	1	7
4	P	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
4	Q	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
5	L	97/99 (98%)	65 (67%)	18 (19%)	14 (14%)	0	0
5	M	97/99 (98%)	65 (67%)	17 (18%)	15 (16%)	0	0
All	All	1620/1640 (99%)	1196 (74%)	296 (18%)	128 (8%)	1	3

5 of 128 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ALA
1	A	71	SER
1	A	101	ALA
1	A	102	SER

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Mol	Chain	Res	Type
1	A	137	ASP

### 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	176/176 (100%)	143 (81%)	33 (19%)	1 9
1	C	176/176 (100%)	145 (82%)	31 (18%)	2 10
2	B	200/200 (100%)	155 (78%)	45 (22%)	1 5
2	D	200/200 (100%)	154 (77%)	46 (23%)	1 5
3	H	232/232 (100%)	197 (85%)	35 (15%)	3 14
3	I	232/232 (100%)	196 (84%)	36 (16%)	2 13
4	P	8/8 (100%)	7 (88%)	1 (12%)	4 20
4	Q	8/8 (100%)	7 (88%)	1 (12%)	4 20
5	L	94/94 (100%)	75 (80%)	19 (20%)	1 7
5	M	94/94 (100%)	74 (79%)	20 (21%)	1 6
All	All	1420/1420 (100%)	1153 (81%)	267 (19%)	1 9

5 of 267 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	132	THR
3	I	213	ILE
5	M	68	THR
3	H	127	ASN
3	H	114	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	136	GLN
5	M	17	ASN

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Mol	Chain	Res	Type
2	D	28	ASN
4	Q	2	GLN
3	I	174	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](#)

There are no ligands in this entry.

### 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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.