



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:19 PM UTC

PDB ID : 4D0D / pdb_00004d0d
Title : COMPLEX OF A B2 CHICKEN MHC CLASS I MOLECULE AND A 8MER CHICKEN PEPTIDE
Authors : Chappell, P.E.; Roversi, P.; Harrison, M.C.; Mears, L.E.; Kaufman, J.F.; Lea, S.M.
Deposited on : 2014-04-25
Resolution : 3.13 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 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

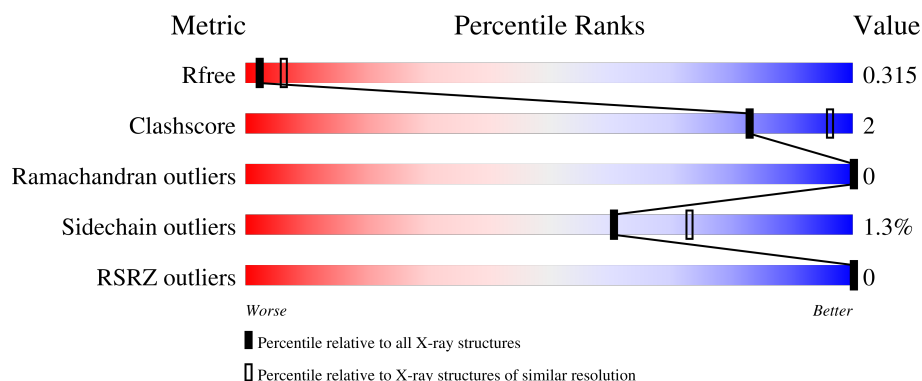
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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.



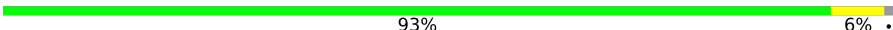
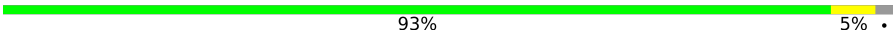
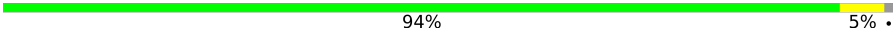
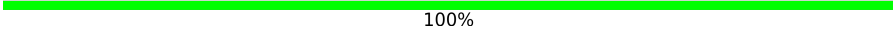
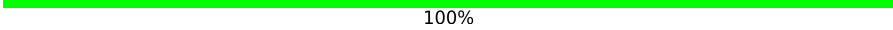
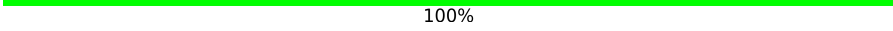
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	310	 81% 8% 11%
1	D	310	 80% 7% 12%
1	G	310	 79% 8% 13%
1	J	310	 79% 10% 12%
2	B	98	 91% 7%

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Mol	Chain	Length	Quality of chain
2	E	98	 93% 6% •
2	H	98	 93% 5% •
2	K	98	 94% 5% •
3	C	8	 100%
3	F	8	 100%
3	I	8	 100%
3	L	8	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12111 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 MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I GLY-COPROTEIN HAPLOTYPE B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2214	1396	394	416	8			
1	D	272	Total	C	N	O	S	0	0	0
			2193	1385	388	412	8			
1	G	270	Total	C	N	O	S	0	0	0
			2177	1375	386	408	8			
1	J	274	Total	C	N	O	S	0	0	0
			2210	1394	393	415	8			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	ARG	-	expression tag	UNP O46789
A	274	SER	-	expression tag	UNP O46789
A	275	GLY	-	expression tag	UNP O46789
A	276	GLY	-	expression tag	UNP O46789
A	277	GLY	-	expression tag	UNP O46789
A	278	LEU	-	expression tag	UNP O46789
A	279	ASN	-	expression tag	UNP O46789
A	280	ASP	-	expression tag	UNP O46789
A	281	ILE	-	expression tag	UNP O46789
A	282	PHE	-	expression tag	UNP O46789
A	283	GLU	-	expression tag	UNP O46789
A	284	ALA	-	expression tag	UNP O46789
A	285	GLN	-	expression tag	UNP O46789
A	286	LYS	-	expression tag	UNP O46789
A	287	ILE	-	expression tag	UNP O46789
A	288	GLU	-	expression tag	UNP O46789
A	289	TRP	-	expression tag	UNP O46789
A	290	HIS	-	expression tag	UNP O46789
A	291	GLU	-	expression tag	UNP O46789
A	292	ASN	-	expression tag	UNP O46789

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Chain	Residue	Modelled	Actual	Comment	Reference
A	293	SER	-	expression tag	UNP O46789
A	294	SER	-	expression tag	UNP O46789
A	295	SER	-	expression tag	UNP O46789
A	296	VAL	-	expression tag	UNP O46789
A	297	ASP	-	expression tag	UNP O46789
A	298	LYS	-	expression tag	UNP O46789
A	299	LEU	-	expression tag	UNP O46789
A	300	ALA	-	expression tag	UNP O46789
A	301	ALA	-	expression tag	UNP O46789
A	302	ALA	-	expression tag	UNP O46789
A	303	LEU	-	expression tag	UNP O46789
A	304	GLU	-	expression tag	UNP O46789
A	305	HIS	-	expression tag	UNP O46789
A	306	HIS	-	expression tag	UNP O46789
A	307	HIS	-	expression tag	UNP O46789
A	308	HIS	-	expression tag	UNP O46789
A	309	HIS	-	expression tag	UNP O46789
A	310	HIS	-	expression tag	UNP O46789
D	273	ARG	-	expression tag	UNP O46789
D	274	SER	-	expression tag	UNP O46789
D	275	GLY	-	expression tag	UNP O46789
D	276	GLY	-	expression tag	UNP O46789
D	277	GLY	-	expression tag	UNP O46789
D	278	LEU	-	expression tag	UNP O46789
D	279	ASN	-	expression tag	UNP O46789
D	280	ASP	-	expression tag	UNP O46789
D	281	ILE	-	expression tag	UNP O46789
D	282	PHE	-	expression tag	UNP O46789
D	283	GLU	-	expression tag	UNP O46789
D	284	ALA	-	expression tag	UNP O46789
D	285	GLN	-	expression tag	UNP O46789
D	286	LYS	-	expression tag	UNP O46789
D	287	ILE	-	expression tag	UNP O46789
D	288	GLU	-	expression tag	UNP O46789
D	289	TRP	-	expression tag	UNP O46789
D	290	HIS	-	expression tag	UNP O46789
D	291	GLU	-	expression tag	UNP O46789
D	292	ASN	-	expression tag	UNP O46789
D	293	SER	-	expression tag	UNP O46789
D	294	SER	-	expression tag	UNP O46789
D	295	SER	-	expression tag	UNP O46789
D	296	VAL	-	expression tag	UNP O46789

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Chain	Residue	Modelled	Actual	Comment	Reference
D	297	ASP	-	expression tag	UNP O46789
D	298	LYS	-	expression tag	UNP O46789
D	299	LEU	-	expression tag	UNP O46789
D	300	ALA	-	expression tag	UNP O46789
D	301	ALA	-	expression tag	UNP O46789
D	302	ALA	-	expression tag	UNP O46789
D	303	LEU	-	expression tag	UNP O46789
D	304	GLU	-	expression tag	UNP O46789
D	305	HIS	-	expression tag	UNP O46789
D	306	HIS	-	expression tag	UNP O46789
D	307	HIS	-	expression tag	UNP O46789
D	308	HIS	-	expression tag	UNP O46789
D	309	HIS	-	expression tag	UNP O46789
D	310	HIS	-	expression tag	UNP O46789
G	273	ARG	-	expression tag	UNP O46789
G	274	SER	-	expression tag	UNP O46789
G	275	GLY	-	expression tag	UNP O46789
G	276	GLY	-	expression tag	UNP O46789
G	277	GLY	-	expression tag	UNP O46789
G	278	LEU	-	expression tag	UNP O46789
G	279	ASN	-	expression tag	UNP O46789
G	280	ASP	-	expression tag	UNP O46789
G	281	ILE	-	expression tag	UNP O46789
G	282	PHE	-	expression tag	UNP O46789
G	283	GLU	-	expression tag	UNP O46789
G	284	ALA	-	expression tag	UNP O46789
G	285	GLN	-	expression tag	UNP O46789
G	286	LYS	-	expression tag	UNP O46789
G	287	ILE	-	expression tag	UNP O46789
G	288	GLU	-	expression tag	UNP O46789
G	289	TRP	-	expression tag	UNP O46789
G	290	HIS	-	expression tag	UNP O46789
G	291	GLU	-	expression tag	UNP O46789
G	292	ASN	-	expression tag	UNP O46789
G	293	SER	-	expression tag	UNP O46789
G	294	SER	-	expression tag	UNP O46789
G	295	SER	-	expression tag	UNP O46789
G	296	VAL	-	expression tag	UNP O46789
G	297	ASP	-	expression tag	UNP O46789
G	298	LYS	-	expression tag	UNP O46789
G	299	LEU	-	expression tag	UNP O46789
G	300	ALA	-	expression tag	UNP O46789

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Chain	Residue	Modelled	Actual	Comment	Reference
G	301	ALA	-	expression tag	UNP O46789
G	302	ALA	-	expression tag	UNP O46789
G	303	LEU	-	expression tag	UNP O46789
G	304	GLU	-	expression tag	UNP O46789
G	305	HIS	-	expression tag	UNP O46789
G	306	HIS	-	expression tag	UNP O46789
G	307	HIS	-	expression tag	UNP O46789
G	308	HIS	-	expression tag	UNP O46789
G	309	HIS	-	expression tag	UNP O46789
G	310	HIS	-	expression tag	UNP O46789
J	273	ARG	-	expression tag	UNP O46789
J	274	SER	-	expression tag	UNP O46789
J	275	GLY	-	expression tag	UNP O46789
J	276	GLY	-	expression tag	UNP O46789
J	277	GLY	-	expression tag	UNP O46789
J	278	LEU	-	expression tag	UNP O46789
J	279	ASN	-	expression tag	UNP O46789
J	280	ASP	-	expression tag	UNP O46789
J	281	ILE	-	expression tag	UNP O46789
J	282	PHE	-	expression tag	UNP O46789
J	283	GLU	-	expression tag	UNP O46789
J	284	ALA	-	expression tag	UNP O46789
J	285	GLN	-	expression tag	UNP O46789
J	286	LYS	-	expression tag	UNP O46789
J	287	ILE	-	expression tag	UNP O46789
J	288	GLU	-	expression tag	UNP O46789
J	289	TRP	-	expression tag	UNP O46789
J	290	HIS	-	expression tag	UNP O46789
J	291	GLU	-	expression tag	UNP O46789
J	292	ASN	-	expression tag	UNP O46789
J	293	SER	-	expression tag	UNP O46789
J	294	SER	-	expression tag	UNP O46789
J	295	SER	-	expression tag	UNP O46789
J	296	VAL	-	expression tag	UNP O46789
J	297	ASP	-	expression tag	UNP O46789
J	298	LYS	-	expression tag	UNP O46789
J	299	LEU	-	expression tag	UNP O46789
J	300	ALA	-	expression tag	UNP O46789
J	301	ALA	-	expression tag	UNP O46789
J	302	ALA	-	expression tag	UNP O46789
J	303	LEU	-	expression tag	UNP O46789
J	304	GLU	-	expression tag	UNP O46789

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Chain	Residue	Modelled	Actual	Comment	Reference
J	305	HIS	-	expression tag	UNP O46789
J	306	HIS	-	expression tag	UNP O46789
J	307	HIS	-	expression tag	UNP O46789
J	308	HIS	-	expression tag	UNP O46789
J	309	HIS	-	expression tag	UNP O46789
J	310	HIS	-	expression tag	UNP O46789

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	S	0	0	0
			759	486	124	144	5			
2	E	97	Total	C	N	O	S	0	0	0
			771	495	125	146	5			
2	H	96	Total	C	N	O	S	0	0	0
			759	486	124	144	5			
2	K	97	Total	C	N	O	S	0	0	0
			771	495	125	146	5			

- Molecule 3 is a protein called SLP-76 ADAPTOR PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			62	43	9	10			
3	F	8	Total	C	N	O	0	0	0
			62	43	9	10			
3	I	8	Total	C	N	O	0	0	0
			62	43	9	10			
3	L	8	Total	C	N	O	0	0	0
			62	43	9	10			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	D	3	Total	O	0	0
			3	3		
4	E	1	Total	O	0	0
			1	1		

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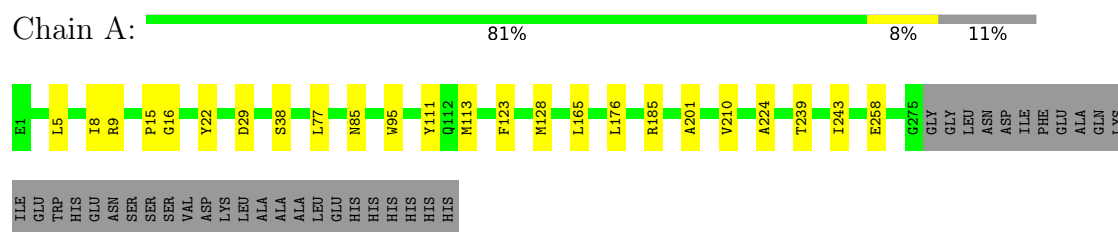
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	O 1	0	0
4	I	1	Total 1	O 1	0	0
4	J	1	Total 1	O 1	0	0

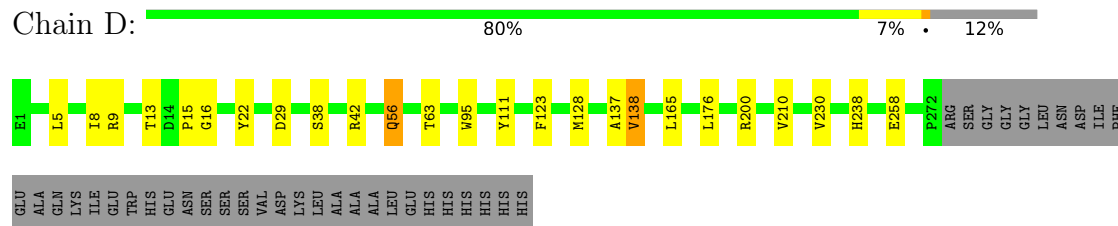
3 Residue-property plots

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 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.

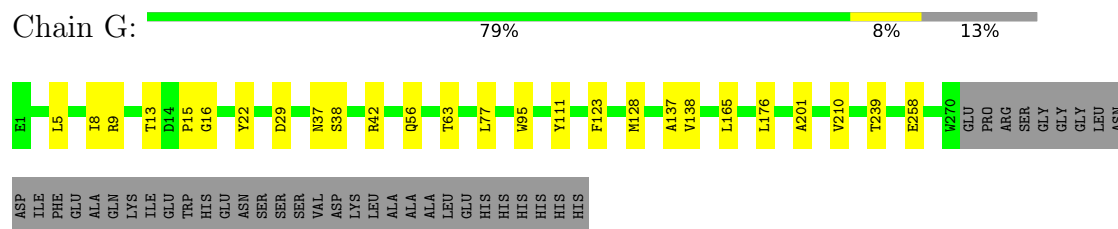
- Molecule 1: MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I GLYCOPROTEIN HAP-LOTYP B2



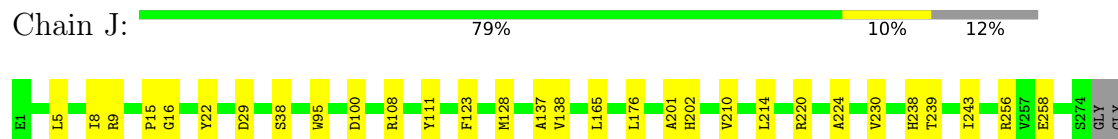
- Molecule 1: MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I GLYCOPROTEIN HAP-LOTYP B2



- Molecule 1: MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I GLYCOPROTEIN HAP-LOTYP B2



- Molecule 1: MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I GLYCOPROTEIN HAP-LOTYP B2



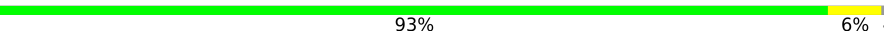
GLY
LEU
ASN
ASP
ILE
PHE
GLU
ALA
GLN
LYS
ILE
GLU
TEP
HIS
GLU
ASN
SER
SER
SER
VAL
ASP
LYS
LEU
ALA
ALA
LEU
GLU
HIS
HIS
HIS
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HIS

• Molecule 2: BETA-2-MICROGLOBULIN

Chain B:  91% 7%

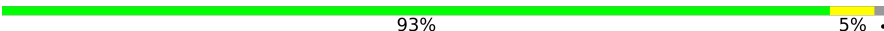
ASP
L2
P13
G28
S35
M39
T60
K80
Y81
E82
E97
PHE

• Molecule 2: BETA-2-MICROGLOBULIN

Chain E:  93% 6%

ASP
L2
G28
S35
E46
T60
E82
F98

• Molecule 2: BETA-2-MICROGLOBULIN

Chain H:  93% 5%

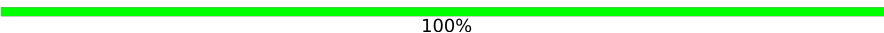
ASP
L2
G28
S35
E46
T60
E82
E97
PHE

• Molecule 2: BETA-2-MICROGLOBULIN

Chain K:  94% 5%

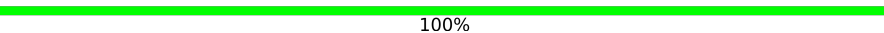
ASP
L2
G28
S35
T60
E82
F98

• Molecule 3: SLP-76 ADAPTOR PROTEIN

Chain C:  100%

There are no outlier residues recorded for this chain.

• Molecule 3: SLP-76 ADAPTOR PROTEIN

Chain F:  100%

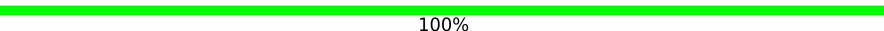
There are no outlier residues recorded for this chain.

• Molecule 3: SLP-76 ADAPTOR PROTEIN

Chain I:  100%

There are no outlier residues recorded for this chain.

• Molecule 3: SLP-76 ADAPTOR PROTEIN

Chain L:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.08Å 92.54Å 223.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.95 – 3.13 81.95 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.1 (81.95-3.13) 86.7 (81.95-3.13)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.292 , 0.299 0.304 , 0.315	Depositor DCC
R_{free} test set	1667 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 7.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.066 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12111	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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

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	0.68	0/2279	1.15	0/3098
1	D	0.69	0/2258	1.16	3/3071 (0.1%)
1	G	0.69	1/2241 (0.0%)	1.16	3/3047 (0.1%)
1	J	0.69	0/2275	1.16	3/3093 (0.1%)
2	B	0.72	0/783	1.05	0/1065
2	E	0.72	0/796	1.07	1/1081 (0.1%)
2	H	0.72	0/783	1.05	0/1065
2	K	0.74	0/796	1.07	0/1081
3	C	0.67	0/63	0.95	0/83
3	F	0.67	0/63	0.95	0/83
3	I	0.67	0/63	0.95	0/83
3	L	0.67	0/63	0.96	0/83
All	All	0.70	1/12463 (0.0%)	1.13	10/16933 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	138	VAL	CA-C	5.43	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	138	VAL	N-CA-CB	7.79	115.41	110.50
1	D	138	VAL	N-CA-CB	7.55	115.26	110.50
1	D	137	ALA	CA-C-N	6.35	124.24	120.24
1	D	137	ALA	C-N-CA	6.35	124.24	120.24
1	G	138	VAL	N-CA-CB	6.33	114.49	110.50
1	G	137	ALA	CA-C-N	5.88	123.94	120.24
1	G	137	ALA	C-N-CA	5.88	123.94	120.24
1	J	137	ALA	CA-C-N	5.66	123.81	120.24
1	J	137	ALA	C-N-CA	5.66	123.81	120.24
2	E	98	PHE	CA-CB-CG	5.61	119.41	113.80

There are no chirality outliers.

There are no planarity outliers.

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	2214	0	2083	12	0
1	D	2193	0	2062	11	0
1	G	2177	0	2049	11	0
1	J	2210	0	2080	14	0
2	B	759	0	721	4	0
2	E	771	0	730	3	0
2	H	759	0	721	3	0
2	K	771	0	730	2	0
3	C	62	0	72	0	0
3	F	62	0	72	0	0
3	I	62	0	72	0	0
3	L	62	0	72	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	3	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
All	All	12111	0	11464	56	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 2.

All (56) 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:9:ARG:HB3	1:A:95:TRP:HB2	1.67	0.76
2:E:46:GLU:HG3	1:G:13:THR:HG22	1.76	0.67
1:D:9:ARG:HB3	1:D:95:TRP:HB2	1.78	0.65
2:H:28:GLY:HA2	2:H:60:THR:HB	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLY:HA2	2:B:60:THR:HB	1.83	0.59
1:J:9:ARG:HB3	1:J:95:TRP:HB2	1.84	0.59
2:K:28:GLY:HA2	2:K:60:THR:HB	1.83	0.59
1:G:9:ARG:HB3	1:G:95:TRP:HB2	1.85	0.59
2:E:28:GLY:HA2	2:E:60:THR:HB	1.84	0.59
1:J:210:VAL:HB	1:J:258:GLU:HB2	1.86	0.58
1:A:210:VAL:HB	1:A:258:GLU:HB2	1.86	0.58
1:D:210:VAL:HB	1:D:258:GLU:HB2	1.86	0.58
2:K:35:SER:HB3	2:K:82:GLU:HB2	1.86	0.57
2:H:35:SER:HB3	2:H:82:GLU:HB2	1.86	0.57
2:E:35:SER:HB3	2:E:82:GLU:HB2	1.86	0.57
1:G:210:VAL:HB	1:G:258:GLU:HB2	1.86	0.57
2:B:35:SER:HB3	2:B:82:GLU:HB2	1.86	0.57
1:A:95:TRP:NE1	1:A:113:MET:HE2	2.21	0.56
1:G:42:ARG:HD2	1:G:63:THR:HG21	1.92	0.52
1:D:42:ARG:HD2	1:D:63:THR:HG21	1.92	0.51
1:J:214:LEU:HD21	1:J:256:ARG:HH21	1.77	0.50
1:A:22:TYR:HB3	1:A:38:SER:HB3	1.94	0.49
2:B:39:MET:HE2	2:B:80:LYS:HB2	1.96	0.48
1:J:22:TYR:HB3	1:J:38:SER:HB3	1.95	0.48
1:D:13:THR:HG22	2:H:46:GLU:HG3	1.95	0.48
1:G:5:LEU:HB2	1:G:165:LEU:HD13	1.96	0.48
1:J:100:ASP:HB2	1:J:108:ARG:HB2	1.95	0.48
1:J:220:ARG:HD3	1:J:243:ILE:HD11	1.95	0.48
1:G:22:TYR:HB3	1:G:38:SER:HB3	1.97	0.47
1:A:5:LEU:HB2	1:A:165:LEU:HD13	1.96	0.47
1:D:5:LEU:HB2	1:D:165:LEU:HD13	1.96	0.47
1:G:201:ALA:HB3	1:G:239:THR:HG22	1.96	0.47
1:J:5:LEU:HB2	1:J:165:LEU:HD13	1.96	0.47
1:A:95:TRP:HE1	1:A:113:MET:HE2	1.81	0.46
1:G:111:TYR:HB3	1:G:123:PHE:HB3	1.99	0.45
1:J:111:TYR:HB3	1:J:123:PHE:HB3	1.99	0.44
1:A:111:TYR:HB3	1:A:123:PHE:HB3	1.99	0.43
1:J:224:ALA:HB2	1:J:243:ILE:HD12	2.00	0.43
1:D:22:TYR:HB3	1:D:38:SER:HB3	2.00	0.43
1:D:111:TYR:HB3	1:D:123:PHE:HB3	1.99	0.43
1:A:185:ARG:HD2	2:B:13:PRO:HB3	2.01	0.43
1:J:15:PRO:N	1:J:16:GLY:HA2	2.34	0.43
1:J:230:VAL:HG23	1:J:238:HIS:HB3	2.01	0.42
1:D:15:PRO:N	1:D:16:GLY:HA2	2.34	0.42
1:D:56:GLN:HG2	1:G:56:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:PRO:N	1:G:16:GLY:HA2	2.34	0.42
1:J:201:ALA:HB3	1:J:239:THR:HG22	2.00	0.42
1:A:15:PRO:N	1:A:16:GLY:HA2	2.34	0.42
1:A:29:ASP:HB2	1:A:176:LEU:HD22	2.03	0.41
1:G:29:ASP:HB2	1:G:176:LEU:HD22	2.02	0.41
1:A:201:ALA:HB3	1:A:239:THR:HG22	2.02	0.41
1:A:224:ALA:HB2	1:A:243:ILE:HD12	2.03	0.41
1:J:29:ASP:HB2	1:J:176:LEU:HD22	2.03	0.41
1:D:29:ASP:HB2	1:D:176:LEU:HD22	2.03	0.40
1:D:230:VAL:HG23	1:D:238:HIS:HB3	2.02	0.40
1:J:202:HIS:HA	1:J:238:HIS:ND1	2.36	0.40

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	273/310 (88%)	262 (96%)	11 (4%)	0	100	100
1	D	270/310 (87%)	259 (96%)	11 (4%)	0	100	100
1	G	268/310 (86%)	255 (95%)	13 (5%)	0	100	100
1	J	272/310 (88%)	259 (95%)	13 (5%)	0	100	100
2	B	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
2	E	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
2	H	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
2	K	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	F	6/8 (75%)	6 (100%)	0	0	100	100
3	I	6/8 (75%)	6 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	6/8 (75%)	6 (100%)	0	0	100	100
All	All	1485/1664 (89%)	1430 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	224/253 (88%)	220 (98%)	4 (2%)	51	69
1	D	222/253 (88%)	217 (98%)	5 (2%)	44	66
1	G	220/253 (87%)	216 (98%)	4 (2%)	51	69
1	J	224/253 (88%)	222 (99%)	2 (1%)	70	77
2	B	84/86 (98%)	84 (100%)	0	100	100
2	E	85/86 (99%)	85 (100%)	0	100	100
2	H	84/86 (98%)	84 (100%)	0	100	100
2	K	85/86 (99%)	84 (99%)	1 (1%)	63	74
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
3	I	7/7 (100%)	7 (100%)	0	100	100
3	L	7/7 (100%)	7 (100%)	0	100	100
All	All	1256/1384 (91%)	1240 (99%)	16 (1%)	61	73

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	77	LEU
1	A	85	ASN
1	A	128	MET
1	D	8	ILE

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Mol	Chain	Res	Type
1	D	56	GLN
1	D	128	MET
1	D	138	VAL
1	D	200	ARG
1	G	8	ILE
1	G	37	ASN
1	G	77	LEU
1	G	128	MET
1	J	8	ILE
1	J	128	MET
2	K	2	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	202	HIS
1	A	232	ASN
1	A	238	HIS
1	D	86	GLN
1	D	225	HIS
2	E	30	HIS
2	H	7	GLN
2	H	30	HIS
2	H	49	GLN
2	H	66	HIS
1	J	71	GLN
1	J	202	HIS
1	J	232	ASN
1	J	238	HIS

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 [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 [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	275/310 (88%)	-1.47	0 100 100	26, 40, 53, 73	0
1	D	272/310 (87%)	-1.46	0 100 100	26, 44, 58, 68	0
1	G	270/310 (87%)	-1.42	0 100 100	26, 44, 63, 73	0
1	J	274/310 (88%)	-1.42	0 100 100	31, 49, 65, 74	0
2	B	96/98 (97%)	-1.37	0 100 100	46, 56, 69, 92	0
2	E	97/98 (98%)	-1.53	0 100 100	24, 37, 47, 52	0
2	H	96/98 (97%)	-1.47	0 100 100	35, 44, 59, 66	0
2	K	97/98 (98%)	-1.32	0 100 100	52, 66, 81, 85	0
3	C	8/8 (100%)	-1.46	0 100 100	37, 38, 47, 52	0
3	F	8/8 (100%)	-1.59	0 100 100	35, 36, 45, 49	0
3	I	8/8 (100%)	-1.50	0 100 100	34, 35, 45, 49	0
3	L	8/8 (100%)	-1.48	0 100 100	38, 40, 51, 55	0
All	All	1509/1664 (90%)	-1.44	0 100 100	24, 46, 66, 92	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.