



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:16 AM UTC

PDB ID : 5GTM / pdb_00005gtm
Title : Modified human MxA, nucleotide-free form
Authors : Chen, Y.; Gao, S.
Deposited on : 2016-08-22
Resolution : 2.90 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

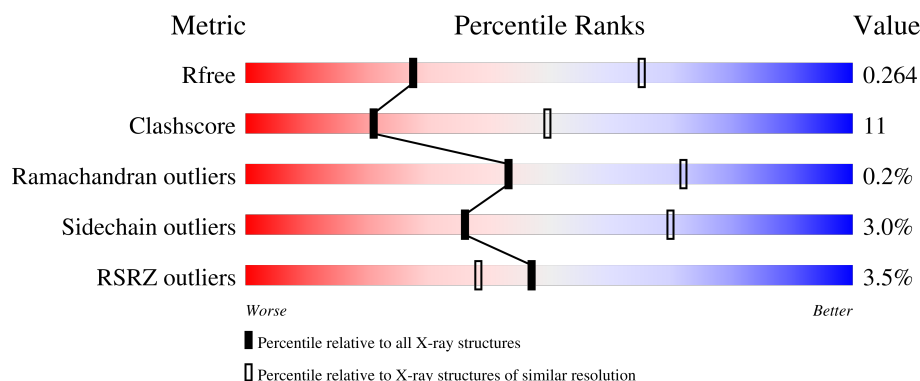
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	601	4% 60% 26% 13%
1	B	601	2% 64% 22% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8454 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 Interferon-induced GTP-binding protein Mx1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4229	2677	728	810	14			
1	B	522	Total	C	N	O	S	0	0	0
			4222	2666	730	812	14			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	376	SER	ILE	engineered mutation	UNP P20591
A	379	ILE	VAL	variant	UNP P20591
A	440	ALA	TYR	engineered mutation	UNP P20591
A	441	ALA	ARG	engineered mutation	UNP P20591
A	442	ALA	GLY	engineered mutation	UNP P20591
A	443	ALA	ARG	engineered mutation	UNP P20591
A	527	ASP	MET	engineered mutation	UNP P20591
A	?	-	CYS	deletion	UNP P20591
A	?	-	GLN	deletion	UNP P20591
A	?	-	ASP	deletion	UNP P20591
A	?	-	GLN	deletion	UNP P20591
A	?	-	VAL	deletion	UNP P20591
A	?	-	TYR	deletion	UNP P20591
A	?	-	ARG	deletion	UNP P20591
A	?	-	GLY	deletion	UNP P20591
A	?	-	ALA	deletion	UNP P20591
A	?	-	LEU	deletion	UNP P20591
A	?	-	GLN	deletion	UNP P20591
A	?	-	LYS	deletion	UNP P20591
A	?	-	VAL	deletion	UNP P20591
A	?	-	ARG	deletion	UNP P20591
A	?	-	GLU	deletion	UNP P20591
A	?	-	LYS	deletion	UNP P20591
A	?	-	GLU	deletion	UNP P20591
A	?	-	LEU	deletion	UNP P20591

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P20591
A	?	-	GLU	deletion	UNP P20591
A	?	-	GLU	deletion	UNP P20591
A	?	-	LYS	deletion	UNP P20591
A	?	-	LYS	deletion	UNP P20591
A	?	-	LYS	deletion	UNP P20591
A	?	-	LYS	deletion	UNP P20591
A	?	-	SER	deletion	UNP P20591
A	?	-	TRP	deletion	UNP P20591
A	?	-	ASP	deletion	UNP P20591
A	?	-	PHE	deletion	UNP P20591
A	614	SER	LYS	engineered mutation	UNP P20591
A	617	SER	LEU	engineered mutation	UNP P20591
A	620	SER	LEU	engineered mutation	UNP P20591
B	376	SER	ILE	engineered mutation	UNP P20591
B	379	ILE	VAL	variant	UNP P20591
B	440	ALA	TYR	engineered mutation	UNP P20591
B	441	ALA	ARG	engineered mutation	UNP P20591
B	442	ALA	GLY	engineered mutation	UNP P20591
B	443	ALA	ARG	engineered mutation	UNP P20591
B	527	ASP	MET	engineered mutation	UNP P20591
B	?	-	CYS	deletion	UNP P20591
B	?	-	GLN	deletion	UNP P20591
B	?	-	ASP	deletion	UNP P20591
B	?	-	GLN	deletion	UNP P20591
B	?	-	VAL	deletion	UNP P20591
B	?	-	TYR	deletion	UNP P20591
B	?	-	ARG	deletion	UNP P20591
B	?	-	GLY	deletion	UNP P20591
B	?	-	ALA	deletion	UNP P20591
B	?	-	LEU	deletion	UNP P20591
B	?	-	GLN	deletion	UNP P20591
B	?	-	LYS	deletion	UNP P20591
B	?	-	VAL	deletion	UNP P20591
B	?	-	ARG	deletion	UNP P20591
B	?	-	GLU	deletion	UNP P20591
B	?	-	LYS	deletion	UNP P20591
B	?	-	GLU	deletion	UNP P20591
B	?	-	LEU	deletion	UNP P20591
B	?	-	GLU	deletion	UNP P20591
B	?	-	GLU	deletion	UNP P20591
B	?	-	GLU	deletion	UNP P20591

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP P20591
B	?	-	LYS	deletion	UNP P20591
B	?	-	LYS	deletion	UNP P20591
B	?	-	LYS	deletion	UNP P20591
B	?	-	SER	deletion	UNP P20591
B	?	-	TRP	deletion	UNP P20591
B	?	-	ASP	deletion	UNP P20591
B	?	-	PHE	deletion	UNP P20591
B	614	SER	LYS	engineered mutation	UNP P20591
B	617	SER	LEU	engineered mutation	UNP P20591
B	620	SER	LEU	engineered mutation	UNP P20591

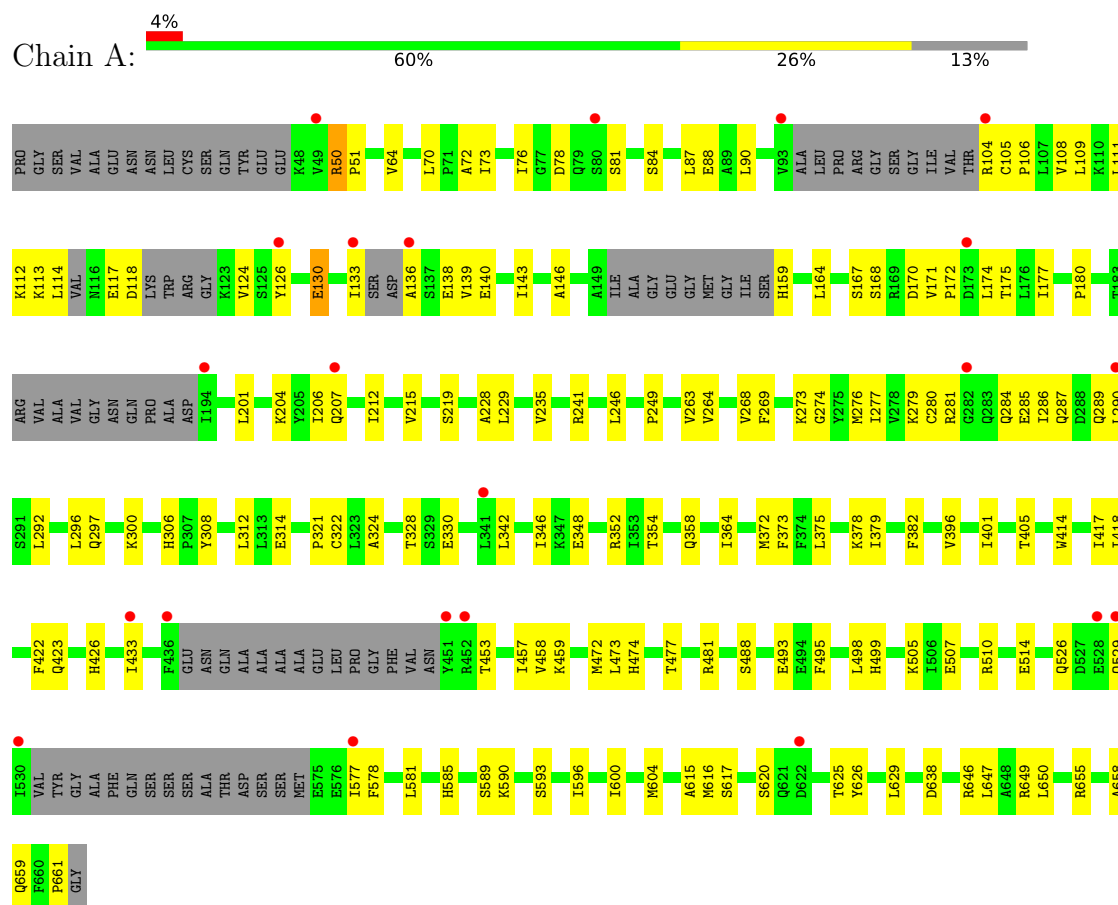
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0
2	B	2	Total O 2 2	0	0

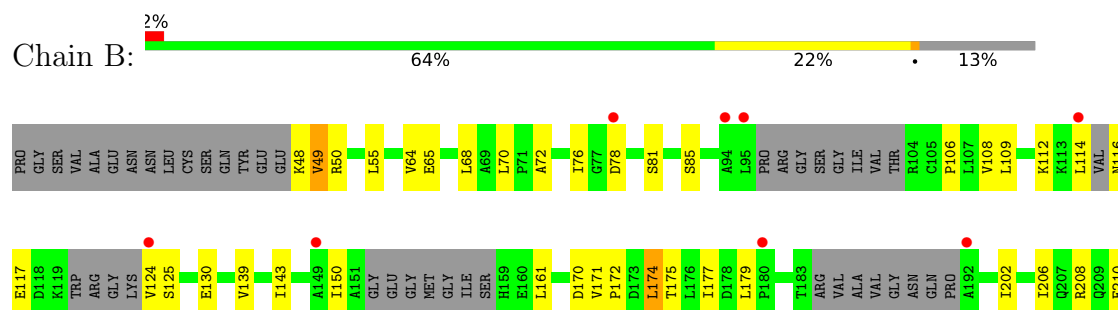
3 Residue-property plots

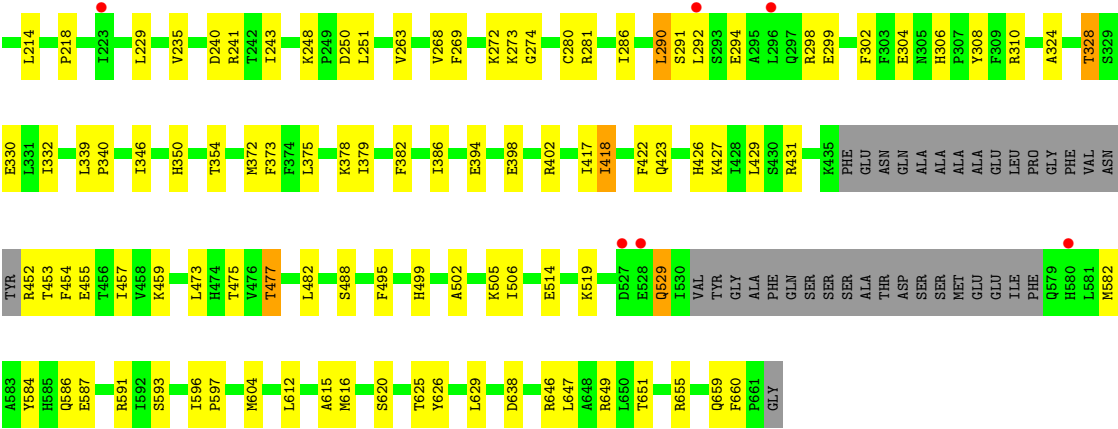
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Interferon-induced GTP-binding protein Mx1



• Molecule 1: Interferon-induced GTP-binding protein Mx1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.18Å 60.16Å 153.92Å 90.00° 98.62° 90.00°	Depositor
Resolution (Å)	39.20 – 2.90 39.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.20-2.90) 98.8 (39.20-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.204 , 0.263 0.210 , 0.264	Depositor DCC
R_{free} test set	2070 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8454	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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	0.64	1/4286 (0.0%)	0.99	10/5759 (0.2%)
1	B	0.64	0/4277	1.01	6/5750 (0.1%)
All	All	0.64	1/8563 (0.0%)	1.00	16/11509 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	596	ILE	CA-CB	-5.27	1.51	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ASP	N-CA-C	-7.31	99.13	110.17
1	A	364	ILE	CA-C-N	6.45	126.41	119.76
1	A	364	ILE	C-N-CA	6.45	126.41	119.76
1	B	398	GLU	N-CA-C	6.34	119.18	111.82
1	A	274	GLY	N-CA-C	6.33	123.98	112.58
1	B	125	SER	N-CA-C	5.93	118.07	107.80
1	A	526	GLN	N-CA-C	-5.87	106.66	113.88
1	A	280	CYS	N-CA-C	5.74	115.86	108.34
1	A	130	GLU	N-CA-C	5.73	117.78	109.07
1	A	396	VAL	N-CA-C	5.64	116.82	108.65
1	B	274	GLY	N-CA-C	5.51	122.92	112.62
1	A	70	LEU	CA-C-N	5.46	125.77	119.93
1	A	70	LEU	C-N-CA	5.46	125.77	119.93
1	B	70	LEU	CA-C-N	5.34	125.65	119.93
1	B	70	LEU	C-N-CA	5.34	125.65	119.93
1	A	117	GLU	N-CA-C	5.30	117.74	111.33

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	4229	0	4291	105	0
1	B	4222	0	4292	82	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
All	All	8454	0	8583	187	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 11.

All (187) 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:50:ARG:H	1:A:51:PRO:HD2	1.33	0.90
1:A:114:LEU:HD13	1:A:118:ASP:HA	1.60	0.82
1:B:174:LEU:HB2	1:B:328:THR:HG22	1.60	0.82
1:A:477:THR:HG22	1:A:604:MET:HG3	1.64	0.80
1:A:105:CYS:HG	1:A:159:HIS:N	1.79	0.80
1:A:422:PHE:HA	1:A:585:HIS:HE1	1.48	0.79
1:B:268:VAL:HG23	1:B:269:PHE:H	1.49	0.78
1:A:78:ASP:HB3	1:A:81:SER:HB3	1.66	0.77
1:B:206:ILE:HG22	1:B:235:VAL:HG11	1.65	0.77
1:B:625:THR:HG22	1:B:629:LEU:HG	1.67	0.77
1:A:249:PRO:HB3	1:A:277:ILE:HD11	1.66	0.76
1:A:174:LEU:HB2	1:A:328:THR:HG22	1.71	0.72
1:A:263:VAL:HG22	1:A:268:VAL:HG21	1.73	0.69
1:A:219:SER:HB3	1:A:246:LEU:HB3	1.74	0.69
1:A:268:VAL:HG23	1:A:269:PHE:H	1.58	0.68
1:B:646:ARG:HG2	1:B:649:ARG:HH21	1.58	0.68
1:A:281:ARG:HE	1:A:292:LEU:HD23	1.59	0.68
1:A:422:PHE:HA	1:A:585:HIS:CE1	2.28	0.67
1:A:206:ILE:HG22	1:A:235:VAL:HG11	1.77	0.66
1:A:281:ARG:HH21	1:A:292:LEU:HA	1.62	0.65
1:B:263:VAL:HA	1:B:268:VAL:HG22	1.79	0.64
1:A:50:ARG:N	1:A:51:PRO:HD2	2.10	0.64
1:B:281:ARG:NH2	1:B:290:LEU:O	2.21	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:HD21	1:B:346:ILE:HG12	1.80	0.63
1:B:477:THR:HG22	1:B:604:MET:HG3	1.79	0.63
1:A:458:VAL:HG13	1:A:585:HIS:HD2	1.64	0.62
1:B:114:LEU:HD22	1:B:117:GLU:HB3	1.82	0.61
1:B:250:ASP:HB2	1:B:251:LEU:HD12	1.82	0.61
1:A:505:LYS:HD3	1:A:615:ALA:HB1	1.82	0.60
1:B:263:VAL:HG22	1:B:268:VAL:HG21	1.83	0.60
1:B:473:LEU:O	1:B:477:THR:HG23	2.03	0.59
1:A:382:PHE:CE2	1:A:616:MET:HG3	2.38	0.58
1:A:422:PHE:HD1	1:A:585:HIS:HD1	1.51	0.58
1:A:281:ARG:NH2	1:A:290:LEU:O	2.37	0.58
1:B:324:ALA:O	1:B:328:THR:HG23	2.04	0.58
1:B:81:SER:HA	1:B:218:PRO:HD3	1.85	0.57
1:A:297:GLN:HA	1:A:300:LYS:HE3	1.87	0.57
1:A:378:LYS:HE3	1:A:495:PHE:CE1	2.40	0.57
1:A:105:CYS:SG	1:A:159:HIS:N	2.79	0.56
1:A:625:THR:HG22	1:A:629:LEU:HG	1.85	0.56
1:B:72:ALA:HB1	1:B:177:ILE:HD13	1.87	0.56
1:A:473:LEU:O	1:A:477:THR:HG23	2.06	0.56
1:B:379:ILE:HD13	1:B:616:MET:O	2.05	0.56
1:B:429:LEU:HD23	1:B:582:MET:SD	2.46	0.56
1:A:124:VAL:HG12	1:A:164:LEU:HD13	1.88	0.56
1:B:477:THR:HG21	1:B:514:GLU:HG3	1.88	0.55
1:A:139:VAL:O	1:A:143:ILE:HG13	2.07	0.54
1:A:263:VAL:HA	1:A:268:VAL:HG22	1.88	0.54
1:A:375:LEU:O	1:A:379:ILE:HG13	2.07	0.54
1:B:55:LEU:HD12	1:B:660:PHE:CG	2.42	0.54
1:A:481:ARG:HD3	1:A:510:ARG:HD3	1.90	0.54
1:A:50:ARG:HD2	1:A:112:LYS:HD2	1.89	0.54
1:B:529:GLN:O	1:B:584:TYR:OH	2.24	0.53
1:A:458:VAL:HG13	1:A:585:HIS:CD2	2.43	0.53
1:A:133:ILE:HG21	1:A:136:ALA:N	2.23	0.53
1:A:133:ILE:HD11	1:A:138:GLU:OE1	2.10	0.53
1:B:502:ALA:O	1:B:506:ILE:HG13	2.09	0.53
1:A:109:LEU:O	1:A:175:THR:HA	2.08	0.52
1:B:354:THR:HG22	1:B:647:LEU:HD21	1.90	0.52
1:A:286:ILE:O	1:A:289:GLN:HG2	2.11	0.50
1:B:505:LYS:HD2	1:B:615:ALA:HB1	1.93	0.50
1:A:284:GLN:O	1:A:287:GLN:HG2	2.11	0.50
1:B:306:HIS:CE1	1:B:308:TYR:HB2	2.47	0.50
1:B:372:MET:HE3	1:B:373:PHE:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:VAL:HG13	1:B:50:ARG:H	1.76	0.49
1:B:382:PHE:O	1:B:386:ILE:HG12	2.13	0.49
1:B:620:SER:O	1:B:626:TYR:OH	2.27	0.49
1:B:339:LEU:HB2	1:B:340:PRO:HD3	1.95	0.48
1:B:646:ARG:HG2	1:B:649:ARG:NH2	2.25	0.48
1:A:50:ARG:CD	1:A:112:LYS:HD2	2.42	0.48
1:A:84:SER:O	1:A:88:GLU:HG3	2.13	0.48
1:B:378:LYS:HE3	1:B:495:PHE:CE1	2.48	0.48
1:A:126:TYR:HB3	1:A:146:ALA:HB1	1.96	0.48
1:B:179:LEU:HD13	1:B:202:ILE:HG12	1.96	0.48
1:A:159:HIS:ND1	1:A:159:HIS:O	2.45	0.48
1:A:201:LEU:O	1:A:204:LYS:HB3	2.14	0.48
1:B:109:LEU:O	1:B:175:THR:HA	2.13	0.48
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.67	0.48
1:B:418:ILE:HG12	1:B:593:SER:HB2	1.96	0.48
1:A:324:ALA:O	1:A:328:THR:HG23	2.14	0.47
1:B:429:LEU:HD11	1:B:454:PHE:HB3	1.96	0.47
1:B:235:VAL:CG1	1:B:241:ARG:HH12	2.27	0.47
1:A:620:SER:O	1:A:626:TYR:OH	2.27	0.47
1:A:458:VAL:HG21	1:A:581:LEU:HB3	1.96	0.47
1:A:474:HIS:ND1	1:A:514:GLU:OE2	2.39	0.47
1:A:72:ALA:HB1	1:A:177:ILE:HD13	1.95	0.47
1:B:281:ARG:HD3	1:B:286:ILE:HG12	1.96	0.46
1:A:306:HIS:HE1	1:A:308:TYR:HB2	1.79	0.46
1:B:459:LYS:HE2	1:B:529:GLN:HB2	1.96	0.46
1:B:179:LEU:HD13	1:B:202:ILE:HA	1.97	0.46
1:B:268:VAL:HG23	1:B:269:PHE:N	2.24	0.46
1:B:375:LEU:O	1:B:379:ILE:HG13	2.14	0.46
1:A:481:ARG:HD2	1:A:507:GLU:OE2	2.15	0.46
1:B:427:LYS:HE3	1:B:431:ARG:HD2	1.98	0.46
1:A:50:ARG:H	1:A:51:PRO:CD	2.18	0.46
1:A:249:PRO:HD2	1:A:279:LYS:HD2	1.98	0.46
1:B:214:LEU:HD12	1:B:243:ILE:HB	1.98	0.46
1:B:304:GLU:HA	1:B:310:ARG:HD3	1.98	0.46
1:A:354:THR:O	1:A:358:GLN:HG2	2.16	0.45
1:B:85:SER:OG	1:B:280:CYS:HB3	2.17	0.45
1:A:306:HIS:CE1	1:A:308:TYR:HB2	2.51	0.45
1:B:112:LYS:HE3	1:B:112:LYS:HB3	1.85	0.45
1:A:401:ILE:HD12	1:A:405:THR:HG22	1.98	0.45
1:B:240:ASP:OD1	1:B:272:LYS:HG2	2.17	0.45
1:A:235:VAL:CG1	1:A:241:ARG:HH22	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:THR:O	1:B:457:ILE:HD13	2.17	0.45
1:B:587:GLU:OE2	1:B:591:ARG:NH1	2.38	0.45
1:A:646:ARG:HG2	1:A:649:ARG:HH21	1.82	0.45
1:A:354:THR:HG22	1:A:647:LEU:HD21	1.99	0.45
1:A:112:LYS:O	1:A:167:SER:HA	2.17	0.44
1:A:646:ARG:HA	1:A:649:ARG:HH21	1.82	0.44
1:B:394:GLU:O	1:B:402:ARG:NE	2.50	0.44
1:B:423:GLN:HA	1:B:426:HIS:HB3	1.99	0.44
1:A:372:MET:HE3	1:A:373:PHE:CE1	2.52	0.44
1:A:76:ILE:HD11	1:A:206:ILE:CD1	2.47	0.44
1:A:229:LEU:HD23	1:A:229:LEU:HA	1.75	0.44
1:A:113:LYS:HE3	1:A:171:VAL:O	2.18	0.44
1:A:477:THR:HG21	1:A:514:GLU:HG3	2.00	0.44
1:B:106:PRO:HB2	1:B:161:LEU:HD23	1.99	0.44
1:A:273:LYS:HG2	1:A:330:GLU:CD	2.43	0.44
1:B:422:PHE:CE1	1:B:586:GLN:HG3	2.52	0.44
1:A:285:GLU:HA	1:A:285:GLU:OE1	2.18	0.44
1:A:215:VAL:HG13	1:A:228:ALA:HB1	1.99	0.44
1:A:112:LYS:HA	1:A:112:LYS:HD3	1.67	0.43
1:A:646:ARG:HG2	1:A:649:ARG:NH2	2.33	0.43
1:B:76:ILE:HD11	1:B:206:ILE:HD11	1.99	0.43
1:A:73:ILE:HD13	1:A:212:ILE:HB	1.99	0.43
1:A:658:ALA:O	1:A:661:PRO:HD2	2.19	0.43
1:B:273:LYS:HG2	1:B:330:GLU:CD	2.44	0.43
1:B:281:ARG:HH21	1:B:292:LEU:HD22	1.83	0.43
1:B:647:LEU:O	1:B:651:THR:HG23	2.19	0.43
1:A:87:LEU:HA	1:A:90:LEU:HD12	2.00	0.43
1:A:589:SER:O	1:A:593:SER:N	2.40	0.43
1:B:294:GLU:O	1:B:298:ARG:N	2.49	0.43
1:A:108:VAL:HG22	1:A:177:ILE:HG13	2.01	0.42
1:A:296:LEU:HD11	1:A:321:PRO:HG3	2.01	0.42
1:A:453:THR:O	1:A:457:ILE:HG12	2.18	0.42
1:A:459:LYS:NZ	1:A:529:GLN:HG3	2.34	0.42
1:A:581:LEU:HD23	1:A:581:LEU:HA	1.75	0.42
1:B:427:LYS:O	1:B:431:ARG:HB2	2.20	0.42
1:A:109:LEU:HD22	1:A:111:LEU:HD21	1.99	0.42
1:A:104:ARG:O	1:A:180:PRO:HG3	2.20	0.42
1:A:207:GLN:HA	1:A:235:VAL:CG1	2.50	0.42
1:A:414:TRP:CZ2	1:A:418:ILE:HD11	2.54	0.42
1:B:612:LEU:O	1:B:616:MET:HG2	2.19	0.42
1:A:114:LEU:HD12	1:A:168:SER:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ILE:HD12	1:A:578:PHE:HD1	1.84	0.42
1:B:76:ILE:HD11	1:B:206:ILE:CD1	2.50	0.42
1:A:264:VAL:HG11	1:A:312:LEU:HD13	2.02	0.42
1:A:498:LEU:HD12	1:A:498:LEU:HA	1.90	0.42
1:A:268:VAL:HG23	1:A:269:PHE:N	2.31	0.42
1:A:379:ILE:HG21	1:A:617:SER:HA	2.01	0.41
1:B:208:ARG:C	1:B:210:GLU:H	2.28	0.41
1:B:139:VAL:O	1:B:143:ILE:HG13	2.20	0.41
1:A:342:LEU:O	1:A:346:ILE:HG13	2.20	0.41
1:B:65:GLU:HG2	1:B:208:ARG:HH12	1.85	0.41
1:B:350:HIS:NE2	1:B:651:THR:HG22	2.36	0.41
1:A:655:ARG:O	1:A:659:GLN:HG3	2.20	0.41
1:A:159:HIS:CD2	1:A:201:LEU:HD13	2.55	0.41
1:A:650:LEU:HD23	1:A:650:LEU:HA	1.85	0.41
1:B:55:LEU:HD12	1:B:660:PHE:CD1	2.55	0.41
1:B:596:ILE:HB	1:B:597:PRO:HD3	2.03	0.41
1:B:50:ARG:HA	1:B:50:ARG:HD2	1.77	0.41
1:A:171:VAL:HG13	1:A:172:PRO:HD2	2.03	0.41
1:A:235:VAL:HG12	1:A:241:ARG:HH22	1.86	0.41
1:A:379:ILE:HD13	1:A:616:MET:O	2.20	0.41
1:B:49:VAL:HG23	1:B:332:ILE:HD11	2.03	0.41
1:B:171:VAL:HG13	1:B:172:PRO:HD2	2.03	0.41
1:A:50:ARG:N	1:A:51:PRO:CD	2.82	0.41
1:A:207:GLN:HG2	1:A:235:VAL:HG22	2.03	0.41
1:B:655:ARG:HE	1:B:659:GLN:NE2	2.19	0.41
1:A:418:ILE:CG2	1:A:589:SER:HB3	2.51	0.41
1:A:423:GLN:O	1:A:426:HIS:HB3	2.21	0.41
1:B:48:LYS:HG2	1:B:49:VAL:N	2.36	0.41
1:B:299:GLU:O	1:B:302:PHE:N	2.53	0.41
1:B:306:HIS:HE1	1:B:308:TYR:HB2	1.85	0.41
1:B:452:ARG:HA	1:B:455:GLU:HB3	2.03	0.40
1:B:625:THR:HG22	1:B:625:THR:O	2.20	0.40
1:A:76:ILE:HD11	1:A:206:ILE:HD11	2.03	0.40
1:A:276:MET:HE1	1:A:322:CYS:HB3	2.04	0.40
1:A:472:MET:HE3	1:A:600:ILE:HD12	2.04	0.40
1:A:488:SER:OG	1:A:499:HIS:ND1	2.44	0.40
1:B:218:PRO:HB3	1:B:248:LYS:HD2	2.04	0.40
1:B:108:VAL:HG22	1:B:177:ILE:HG13	2.04	0.40
1:B:291:SER:HB3	1:B:294:GLU:CD	2.46	0.40
1:A:348:GLU:O	1:A:352:ARG:HG2	2.21	0.40
1:B:488:SER:OG	1:B:499:HIS:ND1	2.45	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	502/601 (84%)	485 (97%)	15 (3%)	2 (0%)	30	59
1	B	506/601 (84%)	488 (96%)	18 (4%)	0	100	100
All	All	1008/1202 (84%)	973 (96%)	33 (3%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	106	PRO

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	475/534 (89%)	465 (98%)	10 (2%)	47	77
1	B	474/534 (89%)	456 (96%)	18 (4%)	29	64
All	All	949/1068 (89%)	921 (97%)	28 (3%)	36	70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	VAL

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Mol	Chain	Res	Type
1	A	130	GLU
1	A	140	GLU
1	A	170	ASP
1	A	314	GLU
1	A	417	ILE
1	A	493	GLU
1	A	577	ILE
1	A	590	LYS
1	A	638	ASP
1	B	49	VAL
1	B	64	VAL
1	B	116	ASN
1	B	124	VAL
1	B	130	GLU
1	B	150	ILE
1	B	170	ASP
1	B	174	LEU
1	B	290	LEU
1	B	328	THR
1	B	417	ILE
1	B	418	ILE
1	B	475	THR
1	B	477	THR
1	B	482	LEU
1	B	519	LYS
1	B	529	GLN
1	B	638	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	B	144	ASN
1	B	461	GLN

5.3.3 RNA ⓘ

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

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	520/601 (86%)	0.09	22 (4%)	40 32	18, 89, 164, 204	0
1	B	522/601 (86%)	0.02	14 (2%)	56 47	22, 77, 154, 195	0
All	All	1042/1202 (86%)	0.05	36 (3%)	47 38	18, 83, 158, 204	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	ALA	5.0
1	B	180	PRO	3.3
1	A	133	ILE	3.3
1	B	95	LEU	3.2
1	A	290	LEU	3.0
1	B	114	LEU	2.9
1	B	296	LEU	2.9
1	B	223	ILE	2.8
1	B	292	LEU	2.7
1	A	126	TYR	2.7
1	A	529	GLN	2.6
1	A	433	ILE	2.5
1	A	80	SER	2.5
1	A	577	ILE	2.5
1	B	124	VAL	2.4
1	A	436	PHE	2.4
1	A	207	GLN	2.4
1	B	580	HIS	2.4
1	B	78	ASP	2.4
1	B	94	ALA	2.4
1	A	194	ILE	2.4
1	A	173	ASP	2.4
1	A	528	GLU	2.4
1	B	528	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	341	LEU	2.2
1	A	622	ASP	2.2
1	A	282	GLY	2.1
1	A	104	ARG	2.1
1	A	452	ARG	2.1
1	A	530	ILE	2.1
1	A	49	VAL	2.1
1	A	93	VAL	2.1
1	B	192	ALA	2.1
1	B	527	ASP	2.1
1	A	451	TYR	2.1
1	B	149	ALA	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 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.