



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2021 – 08:09 AM JST

PDB ID : 7CGA
Title : Crystal structure of human unphosphorylated p38gamma
Authors : Lee, C.C.; Hsu, S.F.; Chen, K.E.; Wang, A.H.J.; Meng, T.C.
Deposited on : 2020-06-30
Resolution : 3.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.20
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

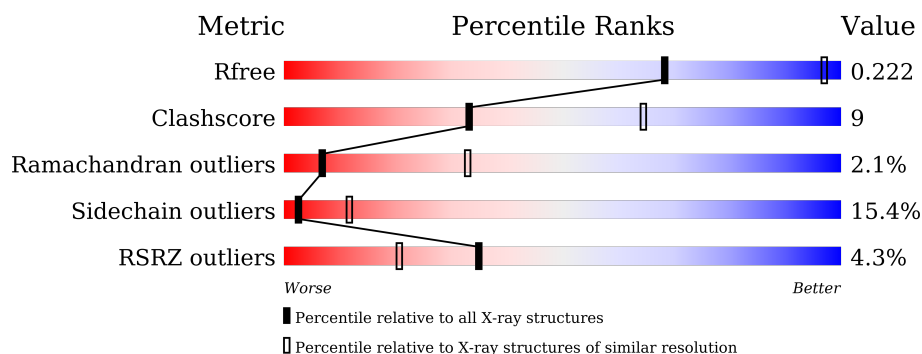
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	348	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	348	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>5% •</div> </div> </div>
1	C	348	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>•</div> </div> </div>
1	D	348	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>5% •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11422 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 Mitogen-activated protein kinase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2798	1787	474	522	15			
1	B	347	Total	C	N	O	S	0	0	0
			2798	1787	474	522	15			
1	C	347	Total	C	N	O	S	0	0	0
			2798	1787	474	522	15			
1	D	347	Total	C	N	O	S	0	0	0
			2798	1787	474	522	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	SER	-	expression tag	UNP P53778
A	7	ASN	-	expression tag	UNP P53778
A	8	ALA	-	expression tag	UNP P53778
B	6	SER	-	expression tag	UNP P53778
B	7	ASN	-	expression tag	UNP P53778
B	8	ALA	-	expression tag	UNP P53778
C	6	SER	-	expression tag	UNP P53778
C	7	ASN	-	expression tag	UNP P53778
C	8	ALA	-	expression tag	UNP P53778
D	6	SER	-	expression tag	UNP P53778
D	7	ASN	-	expression tag	UNP P53778
D	8	ALA	-	expression tag	UNP P53778

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total	O	0	0
			61	61		
2	B	69	Total	O	0	0
			69	69		

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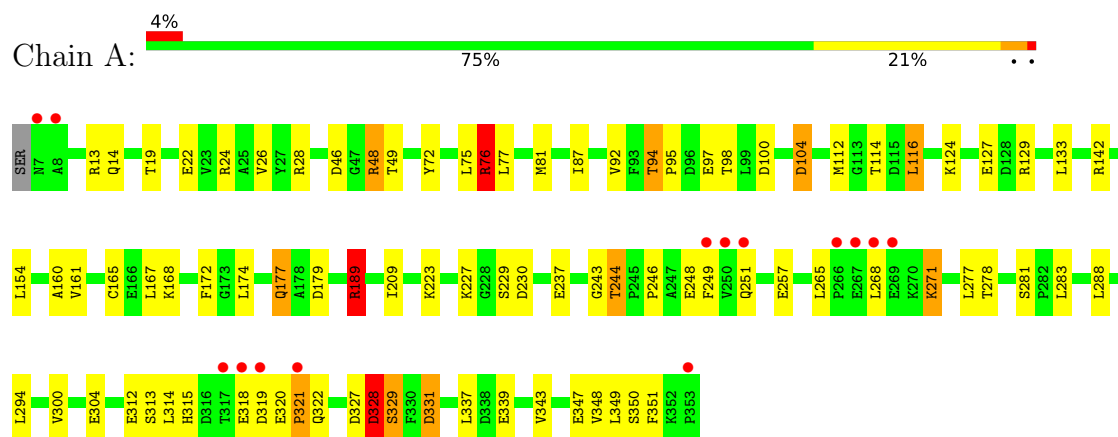
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	57	Total	O	0	0
			57	57		
2	D	43	Total	O	0	0
			43	43		

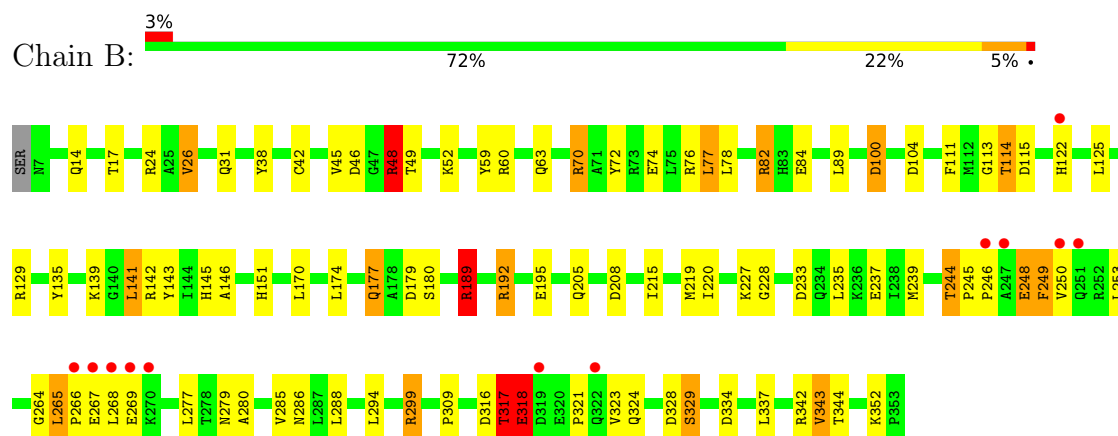
3 Residue-property plots [i](#)

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.

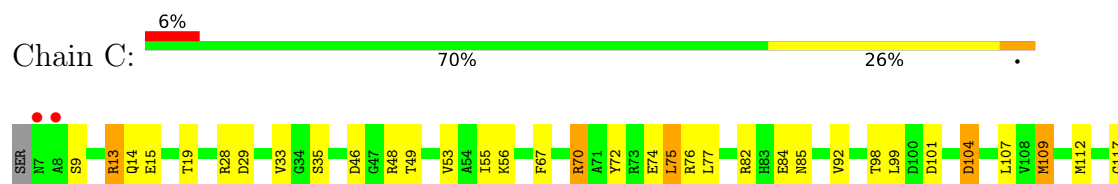
• Molecule 1: Mitogen-activated protein kinase 12

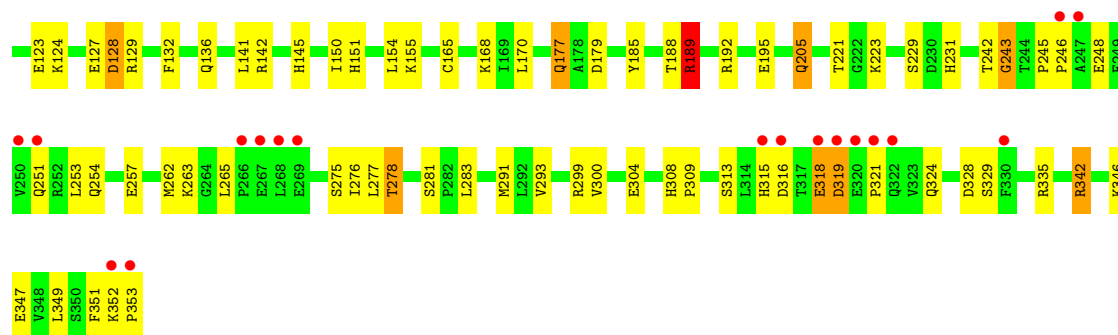


• Molecule 1: Mitogen-activated protein kinase 12

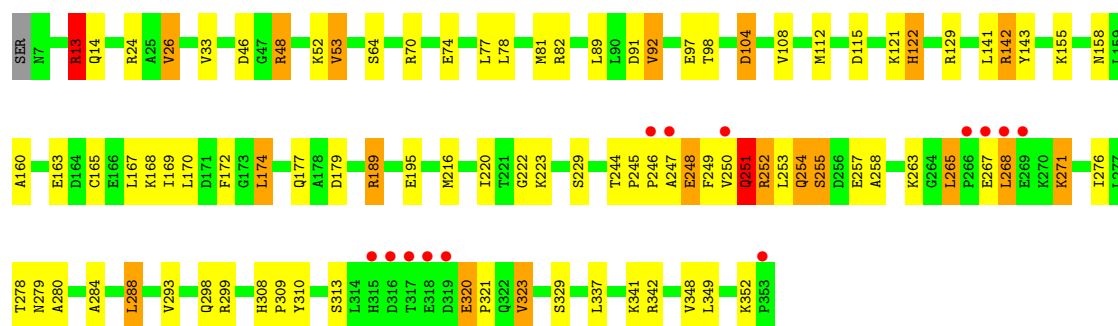


• Molecule 1: Mitogen-activated protein kinase 12





• Molecule 1: Mitogen-activated protein kinase 12



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	183.63Å 183.63Å 294.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 3.15 19.94 – 3.14	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.94-3.15) 99.2 (19.94-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.15Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.160 , 0.218 0.166 , 0.222	Depositor DCC
R_{free} test set	2568 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11422	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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	0.71	0/2858	0.95	3/3862 (0.1%)
1	B	0.70	0/2858	0.95	1/3862 (0.0%)
1	C	0.70	1/2858 (0.0%)	0.94	2/3862 (0.1%)
1	D	0.67	0/2858	0.95	1/3862 (0.0%)
All	All	0.69	1/11432 (0.0%)	0.95	7/15448 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	3
1	D	0	2
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	GLU	CD-OE1	5.52	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	ARG	CG-CD-NE	6.55	125.55	111.80
1	C	104	ASP	CB-CA-C	6.42	123.23	110.40
1	A	76	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	B	189	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	189	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	189	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	76	ARG	CG-CD-NE	5.16	122.63	111.80

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	GLN	Peptide
1	A	328	ASP	Peptide
1	B	170	LEU	Peptide
1	B	318	GLU	Peptide
1	C	117	GLY	Peptide
1	C	316	ASP	Peptide
1	C	328	ASP	Peptide
1	D	169	ILE	Peptide
1	D	320	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2798	0	2783	37	0
1	B	2798	0	2783	58	0
1	C	2798	0	2783	52	0
1	D	2798	0	2783	45	0
2	A	61	0	0	9	0
2	B	69	0	0	9	0
2	C	57	0	0	5	0
2	D	43	0	0	2	0
All	All	11422	0	11132	191	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 9.

All (191) 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:C:189:ARG:HG3	1:C:189:ARG:HH11	1.44	0.82
1:C:99:LEU:HD12	1:C:99:LEU:O	1.83	0.78
1:B:70:ARG:NH1	1:B:74:GLU:OE1	2.19	0.75
1:B:249:PHE:HA	1:B:253:LEU:HD13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:THR:N	2:A:401:HOH:O	2.20	0.73
1:A:81:MET:HE1	1:A:172:PHE:CE2	2.27	0.69
1:B:328:ASP:HB2	2:B:446:HOH:O	1.92	0.69
1:D:248:GLU:O	1:D:251:GLN:O	2.11	0.69
1:B:45:VAL:HG12	1:B:46:ASP:O	1.91	0.69
1:B:227:LYS:O	1:B:237:GLU:HG3	1.93	0.68
1:B:316:ASP:O	1:B:318:GLU:N	2.27	0.68
1:B:122:HIS:HB3	2:B:439:HOH:O	1.94	0.66
1:A:19:THR:HB	2:A:411:HOH:O	1.94	0.66
1:A:321:PRO:HG2	2:A:424:HOH:O	1.95	0.66
1:A:327:ASP:OD1	1:A:329:SER:OG	2.14	0.65
1:B:189:ARG:HG3	1:B:189:ARG:HH11	1.61	0.64
1:B:122:HIS:CB	2:B:439:HOH:O	2.46	0.64
1:B:151:HIS:O	1:B:208:ASP:OD1	2.15	0.64
1:D:81:MET:HE1	1:D:172:PHE:CE1	2.32	0.64
1:C:72:TYR:CZ	1:C:76:ARG:HD2	2.33	0.64
1:A:189:ARG:HH11	1:A:189:ARG:HG3	1.63	0.62
1:C:189:ARG:HH11	1:C:189:ARG:CG	2.10	0.62
1:C:177:GLN:HE21	1:C:179:ASP:H	1.45	0.62
1:A:189:ARG:HH11	1:A:189:ARG:CG	2.13	0.61
1:D:177:GLN:HE22	1:D:179:ASP:HB2	1.65	0.61
1:A:339:GLU:O	1:A:343:VAL:HG23	2.00	0.61
1:A:257:GLU:H	1:A:257:GLU:CD	2.04	0.61
1:B:26:VAL:HG11	1:B:48:ARG:HG3	1.83	0.61
1:C:128:ASP:N	1:C:128:ASP:OD1	2.33	0.60
1:D:245:PRO:HD2	1:D:249:PHE:HD2	1.66	0.60
1:C:189:ARG:HG3	1:C:189:ARG:NH1	2.10	0.60
1:C:353:PRO:HD3	2:C:450:HOH:O	2.01	0.59
1:C:56:LYS:HE3	2:C:418:HOH:O	2.01	0.59
1:B:189:ARG:HH11	1:B:189:ARG:CG	2.16	0.58
1:A:76:ARG:NH2	1:A:331:ASP:OD1	2.35	0.58
1:D:78:LEU:HB3	1:D:89:LEU:HD13	1.84	0.58
1:B:248:GLU:C	1:B:250:VAL:H	2.07	0.57
1:B:244:THR:HG22	1:B:249:PHE:HE2	1.69	0.56
1:D:158:ASN:O	1:D:170:LEU:HB2	2.06	0.56
1:D:112:MET:HB2	1:D:160:ALA:HB1	1.87	0.55
1:C:129:ARG:HD2	1:C:165:CYS:SG	2.46	0.55
1:D:279:ASN:N	1:D:279:ASN:OD1	2.36	0.55
1:A:313:SER:HB2	2:A:438:HOH:O	2.06	0.55
1:B:235:LEU:O	1:B:239:MET:HG2	2.07	0.55
1:C:177:GLN:NE2	1:C:179:ASP:H	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:MET:CE	2:C:408:HOH:O	2.54	0.55
1:C:353:PRO:CD	2:C:450:HOH:O	2.55	0.54
1:B:145:HIS:CD2	1:B:205:GLN:HB3	2.43	0.54
1:C:275:SER:O	1:C:278:THR:HG22	2.07	0.54
1:B:60:ARG:O	1:B:63:GLN:HG2	2.08	0.54
1:A:271:LYS:HE3	1:A:271:LYS:CA	2.37	0.53
1:C:283:LEU:HD11	1:C:309:PRO:HB2	1.89	0.53
1:B:317:THR:O	1:B:318:GLU:HG3	2.07	0.53
1:D:26:VAL:HG21	1:D:48:ARG:CD	2.39	0.53
1:D:70:ARG:NH1	1:D:74:GLU:OE1	2.42	0.53
1:C:141:LEU:HD21	1:C:154:LEU:HD11	1.91	0.53
1:C:72:TYR:CE2	1:C:76:ARG:HD3	2.44	0.53
1:C:145:HIS:CD2	1:C:205:GLN:HG2	2.44	0.53
1:D:104:ASP:HB2	2:D:402:HOH:O	2.08	0.53
1:D:265:LEU:H	1:D:265:LEU:HD22	1.72	0.53
1:D:81:MET:HE3	1:D:172:PHE:CZ	2.44	0.52
1:C:75:LEU:HD12	1:C:75:LEU:O	2.10	0.52
1:D:268:LEU:N	1:D:268:LEU:HD23	2.24	0.52
1:C:150:ILE:HG22	1:C:151:HIS:O	2.10	0.52
1:D:46:ASP:OD1	1:D:48:ARG:NH2	2.43	0.52
1:D:53:VAL:HG13	1:D:108:VAL:HG13	1.92	0.51
1:A:268:LEU:H	1:A:268:LEU:HD23	1.75	0.51
1:D:244:THR:HG1	1:D:249:PHE:HE2	1.58	0.51
1:B:100:ASP:OD1	1:B:100:ASP:N	2.43	0.51
1:C:254:GLN:CG	1:C:254:GLN:O	2.59	0.51
1:D:265:LEU:HD23	1:D:265:LEU:O	2.12	0.50
1:A:112:MET:HB2	1:A:160:ALA:HB1	1.92	0.50
1:C:99:LEU:HD21	1:C:342:ARG:HG3	1.93	0.50
1:A:94:THR:HG22	1:A:348:VAL:HG11	1.93	0.50
1:B:245:PRO:HD2	1:B:249:PHE:CE2	2.46	0.50
1:B:277:LEU:HD13	1:B:288:LEU:HD13	1.93	0.50
1:D:92:VAL:HG22	1:D:348:VAL:HG13	1.93	0.49
1:C:85:ASN:ND2	1:C:136:GLN:HB3	2.27	0.49
1:C:254:GLN:O	1:C:254:GLN:NE2	2.45	0.49
1:D:271:LYS:HG2	1:D:276:ILE:HD11	1.94	0.49
1:C:155:LYS:HD3	1:C:188:THR:HG21	1.95	0.49
1:B:344:THR:HG21	2:B:403:HOH:O	2.12	0.49
1:D:252:ARG:O	1:D:253:LEU:HD12	2.12	0.49
1:A:104:ASP:HB2	2:A:407:HOH:O	2.11	0.49
1:C:221:THR:HG21	1:C:277:LEU:HD23	1.95	0.49
1:D:247:ALA:O	1:D:252:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ASP:HB3	1:D:108:VAL:HB	1.94	0.49
1:B:78:LEU:HB3	1:B:89:LEU:HD13	1.95	0.48
1:B:177:GLN:HE21	1:B:179:ASP:H	1.61	0.48
1:B:244:THR:HG22	1:B:249:PHE:CE2	2.47	0.48
1:B:59:TYR:O	1:B:60:ARG:C	2.51	0.48
1:B:76:ARG:HD2	2:B:406:HOH:O	2.13	0.48
1:A:72:TYR:CE2	1:A:76:ARG:HG3	2.48	0.48
1:D:24:ARG:NH1	1:D:91:ASP:OD1	2.48	0.47
1:B:26:VAL:CG1	1:B:48:ARG:HG3	2.44	0.47
1:A:76:ARG:HH21	1:A:76:ARG:CG	2.27	0.47
1:B:265:LEU:HB2	1:B:266:PRO:HD2	1.97	0.47
1:C:132:PHE:O	1:C:136:GLN:HG3	2.15	0.47
1:C:188:THR:O	1:C:192:ARG:HD3	2.14	0.47
1:D:26:VAL:CG2	1:D:48:ARG:CD	2.93	0.47
1:B:285:VAL:O	1:B:286:ASN:C	2.53	0.47
1:B:143:TYR:O	1:B:146:ALA:HB3	2.15	0.47
1:B:189:ARG:O	1:B:192:ARG:HG2	2.15	0.47
1:B:122:HIS:HB2	2:B:439:HOH:O	2.14	0.46
1:D:189:ARG:HH11	1:D:189:ARG:HG3	1.80	0.46
1:B:177:GLN:NE2	1:B:179:ASP:H	2.14	0.46
1:A:243:GLY:C	2:A:401:HOH:O	2.53	0.46
1:A:177:GLN:NE2	1:A:179:ASP:OD2	2.48	0.46
1:B:82:ARG:HD2	2:B:443:HOH:O	2.16	0.46
1:B:26:VAL:HG11	1:B:48:ARG:CG	2.45	0.46
1:A:46:ASP:OD2	1:A:48:ARG:NH2	2.49	0.46
1:C:46:ASP:OD1	1:C:48:ARG:HD3	2.16	0.46
1:C:195:GLU:OE2	1:C:299:ARG:NH2	2.48	0.46
1:A:87:ILE:HD12	1:A:87:ILE:HA	1.76	0.46
1:B:228:GLY:HA2	1:B:233:ASP:OD2	2.17	0.46
1:A:26:VAL:HG11	1:A:48:ARG:NH2	2.31	0.45
1:A:244:THR:CG2	2:A:447:HOH:O	2.63	0.45
1:B:192:ARG:HH21	1:B:192:ARG:CG	2.29	0.45
1:B:321:PRO:HG3	2:B:417:HOH:O	2.17	0.45
1:C:70:ARG:NH1	1:C:74:GLU:OE1	2.49	0.45
1:D:177:GLN:NE2	1:D:179:ASP:HB2	2.29	0.45
1:D:142:ARG:HD2	1:D:321:PRO:HD3	1.99	0.45
1:D:195:GLU:CD	1:D:299:ARG:HH22	2.21	0.45
1:C:318:GLU:HG3	1:C:319:ASP:N	2.31	0.44
1:D:195:GLU:OE2	1:D:299:ARG:NH2	2.50	0.44
1:C:170:LEU:HD23	1:C:170:LEU:HA	1.86	0.44
1:D:268:LEU:HD12	1:D:271:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:MET:CE	1:D:172:PHE:CZ	3.00	0.44
1:C:55:ILE:HA	1:C:107:LEU:O	2.18	0.44
1:C:112:MET:SD	1:C:168:LYS:HE2	2.57	0.44
1:C:254:GLN:O	1:C:254:GLN:HG3	2.17	0.44
1:C:308:HIS:CG	1:C:309:PRO:HD2	2.53	0.44
1:A:227:LYS:O	1:A:237:GLU:HG3	2.18	0.44
1:B:245:PRO:HD2	1:B:249:PHE:HE2	1.83	0.44
1:B:114:THR:OG1	1:B:115:ASP:N	2.50	0.43
1:C:195:GLU:CD	1:C:299:ARG:HH22	2.20	0.43
1:C:13:ARG:HH21	1:C:13:ARG:HB2	1.83	0.43
1:B:189:ARG:HG3	1:B:189:ARG:NH1	2.32	0.43
1:B:220:ILE:HG21	1:B:280:ALA:HB2	1.99	0.43
1:D:220:ILE:HG21	1:D:280:ALA:HB2	1.99	0.43
1:D:268:LEU:HD23	1:D:268:LEU:H	1.83	0.43
1:B:60:ARG:HD3	1:C:35:SER:OG	2.19	0.43
1:D:293:VAL:HG11	1:D:298:GLN:HB2	2.01	0.43
1:C:300:VAL:HG22	1:C:304:GLU:HB2	2.00	0.43
1:D:143:TYR:CE2	1:D:323:VAL:HG13	2.53	0.43
1:D:216:MET:HG2	1:D:288:LEU:HD11	2.01	0.43
1:B:328:ASP:CB	2:B:446:HOH:O	2.59	0.43
1:C:293:VAL:O	1:C:299:ARG:HD3	2.19	0.43
1:B:26:VAL:HG11	1:B:48:ARG:CD	2.48	0.43
1:B:72:TYR:CE1	1:B:343:VAL:CG1	3.01	0.43
1:B:72:TYR:CZ	1:B:76:ARG:HD3	2.53	0.43
1:C:262:MET:O	1:C:265:LEU:HB2	2.19	0.43
1:A:22:GLU:HB2	1:A:95:PRO:HG3	2.01	0.43
1:B:111:PHE:HE2	1:B:113:GLY:HA2	1.84	0.43
1:D:308:HIS:CG	1:D:309:PRO:HD2	2.53	0.43
1:A:160:ALA:O	1:A:167:LEU:HA	2.19	0.42
1:B:31:GLN:O	1:B:42:CYS:HA	2.19	0.42
1:B:26:VAL:HG11	1:B:48:ARG:HD2	2.00	0.42
1:B:113:GLY:C	1:B:114:THR:HG23	2.39	0.42
1:B:135:TYR:CZ	1:B:139:LYS:HD2	2.54	0.42
1:C:291:MET:O	1:C:299:ARG:HD2	2.19	0.42
1:D:255:SER:HB2	1:D:258:ALA:H	1.84	0.42
1:A:189:ARG:HG3	1:A:189:ARG:NH1	2.30	0.42
1:D:13:ARG:HH21	1:D:13:ARG:CG	2.32	0.42
1:D:284:ALA:HB2	1:D:310:TYR:CE1	2.55	0.42
1:A:300:VAL:HG22	1:A:304:GLU:CB	2.50	0.42
1:C:242:THR:O	1:C:243:GLY:O	2.37	0.42
1:D:174:LEU:HD12	1:D:174:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:CD1	1:A:288:LEU:HD13	2.49	0.42
1:B:38:TYR:HB3	1:B:70:ARG:NH2	2.35	0.42
1:A:116:LEU:HD11	1:A:133:LEU:HD13	2.01	0.42
1:A:209:ILE:HG21	1:A:300:VAL:O	2.20	0.41
1:C:329:SER:HB3	2:C:441:HOH:O	2.20	0.41
1:C:72:TYR:CZ	1:C:76:ARG:CD	3.03	0.41
1:C:75:LEU:HD12	1:C:75:LEU:C	2.41	0.41
1:C:76:ARG:NH1	1:C:347:GLU:OE2	2.53	0.41
1:D:160:ALA:O	1:D:167:LEU:HA	2.20	0.41
1:C:72:TYR:CE2	1:C:76:ARG:CD	3.04	0.41
1:B:195:GLU:CD	1:B:299:ARG:HH22	2.23	0.41
1:A:313:SER:CB	2:A:438:HOH:O	2.65	0.41
1:D:189:ARG:NE	2:D:403:HOH:O	2.50	0.41
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.92	0.41
1:A:347:GLU:HG2	2:A:415:HOH:O	2.21	0.41
1:A:76:ARG:HG3	1:A:76:ARG:HH21	1.85	0.41
1:D:251:GLN:O	1:D:252:ARG:HB2	2.21	0.40
1:A:81:MET:CE	1:A:172:PHE:CE2	3.01	0.40
1:B:77:LEU:HD12	1:B:77:LEU:HA	1.78	0.40
1:B:215:ILE:O	1:B:219:MET:HG3	2.21	0.40
1:C:265:LEU:HD12	1:C:265:LEU:HA	1.94	0.40
1:B:141:LEU:HD22	1:B:145:HIS:CE1	2.57	0.40
1:C:185:TYR:OH	1:C:231:HIS:NE2	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	345/348 (99%)	306 (89%)	31 (9%)	8 (2%)	6	31
1	B	345/348 (99%)	309 (90%)	29 (8%)	7 (2%)	7	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	345/348 (99%)	309 (90%)	27 (8%)	9 (3%)	5	28
1	D	345/348 (99%)	312 (90%)	28 (8%)	5 (1%)	11	43
All	All	1380/1392 (99%)	1236 (90%)	115 (8%)	29 (2%)	7	33

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	317	THR
1	B	318	GLU
1	C	318	GLU
1	D	246	PRO
1	D	254	GLN
1	A	116	LEU
1	A	315	HIS
1	B	48	ARG
1	B	246	PRO
1	B	264	GLY
1	C	123	GLU
1	C	243	GLY
1	C	319	ASP
1	A	124	LYS
1	A	246	PRO
1	B	249	PHE
1	B	329	SER
1	C	246	PRO
1	C	315	HIS
1	A	319	ASP
1	A	328	ASP
1	C	313	SER
1	C	321	PRO
1	D	122	HIS
1	D	251	GLN
1	A	320	GLU
1	A	321	PRO
1	C	245	PRO
1	D	222	GLY

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	300/301 (100%)	252 (84%)	48 (16%)	2	10
1	B	300/301 (100%)	258 (86%)	42 (14%)	3	15
1	C	300/301 (100%)	256 (85%)	44 (15%)	3	13
1	D	300/301 (100%)	249 (83%)	51 (17%)	2	9
All	All	1200/1204 (100%)	1015 (85%)	185 (15%)	2	12

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	14	GLN
1	A	24	ARG
1	A	28	ARG
1	A	48	ARG
1	A	49	THR
1	A	75	LEU
1	A	76	ARG
1	A	77	LEU
1	A	92	VAL
1	A	94	THR
1	A	97	GLU
1	A	98	THR
1	A	100	ASP
1	A	104	ASP
1	A	114	THR
1	A	127	GLU
1	A	129	ARG
1	A	142	ARG
1	A	161	VAL
1	A	165	CYS
1	A	168	LYS
1	A	174	LEU
1	A	177	GLN
1	A	189	ARG
1	A	223	LYS
1	A	229	SER
1	A	230	ASP

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Mol	Chain	Res	Type
1	A	244	THR
1	A	248	GLU
1	A	249	PHE
1	A	265	LEU
1	A	271	LYS
1	A	278	THR
1	A	281	SER
1	A	283	LEU
1	A	294	LEU
1	A	312	GLU
1	A	314	LEU
1	A	318	GLU
1	A	322	GLN
1	A	328	ASP
1	A	329	SER
1	A	331	ASP
1	A	337	LEU
1	A	349	LEU
1	A	350	SER
1	A	351	PHE
1	B	14	GLN
1	B	17	THR
1	B	24	ARG
1	B	26	VAL
1	B	48	ARG
1	B	49	THR
1	B	52	LYS
1	B	70	ARG
1	B	77	LEU
1	B	82	ARG
1	B	84	GLU
1	B	100	ASP
1	B	104	ASP
1	B	114	THR
1	B	125	LEU
1	B	129	ARG
1	B	141	LEU
1	B	142	ARG
1	B	174	LEU
1	B	177	GLN
1	B	180	SER
1	B	189	ARG

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Mol	Chain	Res	Type
1	B	192	ARG
1	B	244	THR
1	B	248	GLU
1	B	265	LEU
1	B	267	GLU
1	B	268	LEU
1	B	269	GLU
1	B	279	ASN
1	B	294	LEU
1	B	299	ARG
1	B	309	PRO
1	B	317	THR
1	B	323	VAL
1	B	324	GLN
1	B	329	SER
1	B	334	ASP
1	B	337	LEU
1	B	342	ARG
1	B	343	VAL
1	B	352	LYS
1	C	9	SER
1	C	13	ARG
1	C	14	GLN
1	C	19	THR
1	C	28	ARG
1	C	29	ASP
1	C	33	VAL
1	C	49	THR
1	C	53	VAL
1	C	67	PHE
1	C	70	ARG
1	C	75	LEU
1	C	77	LEU
1	C	82	ARG
1	C	84	GLU
1	C	92	VAL
1	C	98	THR
1	C	101	ASP
1	C	104	ASP
1	C	109	MET
1	C	124	LYS
1	C	127	GLU

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Mol	Chain	Res	Type
1	C	128	ASP
1	C	142	ARG
1	C	177	GLN
1	C	189	ARG
1	C	205	GLN
1	C	223	LYS
1	C	229	SER
1	C	248	GLU
1	C	251	GLN
1	C	253	LEU
1	C	257	GLU
1	C	263	LYS
1	C	276	ILE
1	C	278	THR
1	C	281	SER
1	C	324	GLN
1	C	335	ARG
1	C	342	ARG
1	C	346	LYS
1	C	349	LEU
1	C	351	PHE
1	C	352	LYS
1	D	13	ARG
1	D	14	GLN
1	D	26	VAL
1	D	33	VAL
1	D	48	ARG
1	D	52	LYS
1	D	53	VAL
1	D	64	SER
1	D	77	LEU
1	D	82	ARG
1	D	92	VAL
1	D	97	GLU
1	D	98	THR
1	D	104	ASP
1	D	115	ASP
1	D	121	LYS
1	D	122	HIS
1	D	129	ARG
1	D	141	LEU
1	D	142	ARG

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Mol	Chain	Res	Type
1	D	155	LYS
1	D	163	GLU
1	D	165	CYS
1	D	168	LYS
1	D	174	LEU
1	D	189	ARG
1	D	223	LYS
1	D	229	SER
1	D	248	GLU
1	D	250	VAL
1	D	251	GLN
1	D	252	ARG
1	D	254	GLN
1	D	255	SER
1	D	257	GLU
1	D	263	LYS
1	D	265	LEU
1	D	267	GLU
1	D	268	LEU
1	D	271	LYS
1	D	278	THR
1	D	288	LEU
1	D	313	SER
1	D	320	GLU
1	D	323	VAL
1	D	329	SER
1	D	337	LEU
1	D	341	LYS
1	D	342	ARG
1	D	349	LEU
1	D	352	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	205	GLN
1	B	177	GLN
1	B	205	GLN
1	B	324	GLN
1	C	131	GLN
1	C	177	GLN

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Mol	Chain	Res	Type
1	C	205	GLN
1	C	324	GLN
1	D	177	GLN
1	D	205	GLN
1	D	324	GLN

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 monosaccharides 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	347/348 (99%)	-0.37	14 (4%)	38 23	39, 61, 122, 210	0
1	B	347/348 (99%)	-0.40	12 (3%)	44 27	42, 59, 122, 206	0
1	C	347/348 (99%)	-0.26	20 (5%)	23 12	46, 63, 136, 186	0
1	D	347/348 (99%)	-0.33	13 (3%)	41 25	41, 61, 133, 184	0
All	All	1388/1392 (99%)	-0.34	59 (4%)	35 21	39, 61, 130, 210	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	VAL	9.6
1	C	319	ASP	7.7
1	B	250	VAL	7.2
1	D	319	ASP	6.1
1	D	269	GLU	5.5
1	C	269	GLU	5.0
1	D	353	PRO	4.9
1	C	250	VAL	4.6
1	A	353	PRO	4.4
1	C	266	PRO	4.2
1	D	250	VAL	4.1
1	B	251	GLN	4.1
1	D	318	GLU	4.0
1	A	319	ASP	4.0
1	B	319	ASP	3.9
1	B	269	GLU	3.9
1	C	320	GLU	3.8
1	B	246	PRO	3.7
1	A	317	THR	3.4
1	C	251	GLN	3.4
1	C	246	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	251	GLN	3.3
1	C	268	LEU	3.2
1	A	7	ASN	3.2
1	A	266	PRO	3.2
1	C	318	GLU	3.2
1	A	267	GLU	3.1
1	B	122	HIS	3.1
1	D	317	THR	3.1
1	C	7	ASN	3.0
1	C	8	ALA	3.0
1	B	266	PRO	2.9
1	B	322	GLN	2.9
1	A	268	LEU	2.9
1	C	315	HIS	2.7
1	B	267	GLU	2.7
1	D	266	PRO	2.7
1	D	316	ASP	2.7
1	C	322	GLN	2.7
1	C	353	PRO	2.6
1	D	246	PRO	2.6
1	A	269	GLU	2.6
1	D	268	LEU	2.6
1	A	321	PRO	2.6
1	C	267	GLU	2.5
1	D	247	ALA	2.4
1	C	330	PHE	2.3
1	C	316	ASP	2.3
1	A	318	GLU	2.3
1	B	270	LYS	2.2
1	A	249	PHE	2.2
1	D	315	HIS	2.2
1	B	268	LEU	2.2
1	C	321	PRO	2.2
1	C	247	ALA	2.2
1	D	267	GLU	2.2
1	A	8	ALA	2.1
1	B	247	ALA	2.1
1	C	352	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.