



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:45 PM UTC

PDB ID : 2PHP / pdb_00002php
Title : Crystal structure of the C-terminal domain of protein MJ0236 (Y236_METJA)
Authors : Eswaramoorthy, S.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-04-11
Resolution : 2.03 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

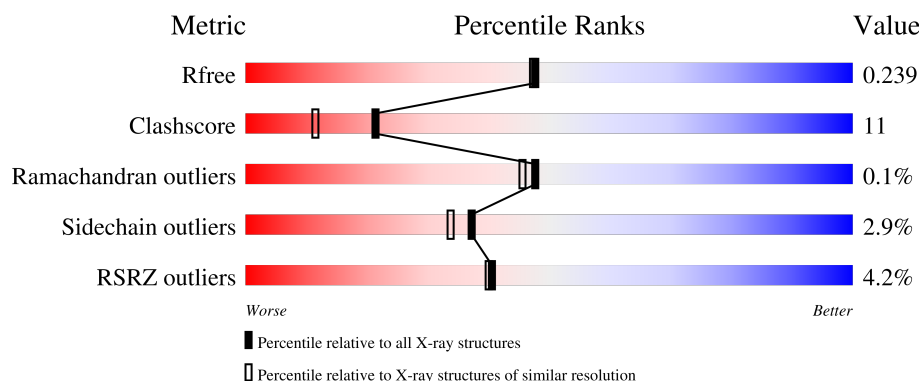
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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 ≥ 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	192	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• 6%</div> </div> </div>
1	B	192	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>
1	D	192	<div> <div>8%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div>• •</div> </div> </div>
1	E	192	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6109 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 Uncharacterized protein MJ0236.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	Se	0	0	0
			1423	925	234	258	2	4			
1	B	186	Total	C	N	O	S	Se	0	0	0
			1462	948	241	267	2	4			
1	D	184	Total	C	N	O	S	Se	0	0	0
			1444	938	237	263	2	4			
1	E	183	Total	C	N	O	S	Se	0	0	0
			1441	935	238	262	2	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	237	MSE	-	cloning artifact	UNP Q57688
A	238	SER	-	cloning artifact	UNP Q57688
A	239	LEU	-	cloning artifact	UNP Q57688
A	261	MSE	MET	modified residue	UNP Q57688
A	333	MSE	MET	modified residue	UNP Q57688
A	366	MSE	MET	modified residue	UNP Q57688
A	395	MSE	MET	modified residue	UNP Q57688
A	421	GLU	-	cloning artifact	UNP Q57688
A	422	GLY	-	cloning artifact	UNP Q57688
A	423	HIS	-	cloning artifact	UNP Q57688
A	424	HIS	-	cloning artifact	UNP Q57688
A	425	HIS	-	cloning artifact	UNP Q57688
A	426	HIS	-	cloning artifact	UNP Q57688
A	427	HIS	-	cloning artifact	UNP Q57688
A	428	HIS	-	cloning artifact	UNP Q57688
B	237	MSE	-	cloning artifact	UNP Q57688
B	238	SER	-	cloning artifact	UNP Q57688
B	239	LEU	-	cloning artifact	UNP Q57688
B	261	MSE	MET	modified residue	UNP Q57688
B	333	MSE	MET	modified residue	UNP Q57688
B	366	MSE	MET	modified residue	UNP Q57688

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Chain	Residue	Modelled	Actual	Comment	Reference
B	395	MSE	MET	modified residue	UNP Q57688
B	421	GLU	-	cloning artifact	UNP Q57688
B	422	GLY	-	cloning artifact	UNP Q57688
B	423	HIS	-	cloning artifact	UNP Q57688
B	424	HIS	-	cloning artifact	UNP Q57688
B	425	HIS	-	cloning artifact	UNP Q57688
B	426	HIS	-	cloning artifact	UNP Q57688
B	427	HIS	-	cloning artifact	UNP Q57688
B	428	HIS	-	cloning artifact	UNP Q57688
D	237	MSE	-	cloning artifact	UNP Q57688
D	238	SER	-	cloning artifact	UNP Q57688
D	239	LEU	-	cloning artifact	UNP Q57688
D	261	MSE	MET	modified residue	UNP Q57688
D	333	MSE	MET	modified residue	UNP Q57688
D	366	MSE	MET	modified residue	UNP Q57688
D	395	MSE	MET	modified residue	UNP Q57688
D	421	GLU	-	cloning artifact	UNP Q57688
D	422	GLY	-	cloning artifact	UNP Q57688
D	423	HIS	-	cloning artifact	UNP Q57688
D	424	HIS	-	cloning artifact	UNP Q57688
D	425	HIS	-	cloning artifact	UNP Q57688
D	426	HIS	-	cloning artifact	UNP Q57688
D	427	HIS	-	cloning artifact	UNP Q57688
D	428	HIS	-	cloning artifact	UNP Q57688
E	237	MSE	-	cloning artifact	UNP Q57688
E	238	SER	-	cloning artifact	UNP Q57688
E	239	LEU	-	cloning artifact	UNP Q57688
E	261	MSE	MET	modified residue	UNP Q57688
E	333	MSE	MET	modified residue	UNP Q57688
E	366	MSE	MET	modified residue	UNP Q57688
E	395	MSE	MET	modified residue	UNP Q57688
E	421	GLU	-	cloning artifact	UNP Q57688
E	422	GLY	-	cloning artifact	UNP Q57688
E	423	HIS	-	cloning artifact	UNP Q57688
E	424	HIS	-	cloning artifact	UNP Q57688
E	425	HIS	-	cloning artifact	UNP Q57688
E	426	HIS	-	cloning artifact	UNP Q57688
E	427	HIS	-	cloning artifact	UNP Q57688
E	428	HIS	-	cloning artifact	UNP Q57688

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Cl 3	0	0
2	B	3	Total 3	Cl 3	0	0
2	D	1	Total 1	Cl 1	0	0
2	E	2	Total 2	Cl 2	0	0

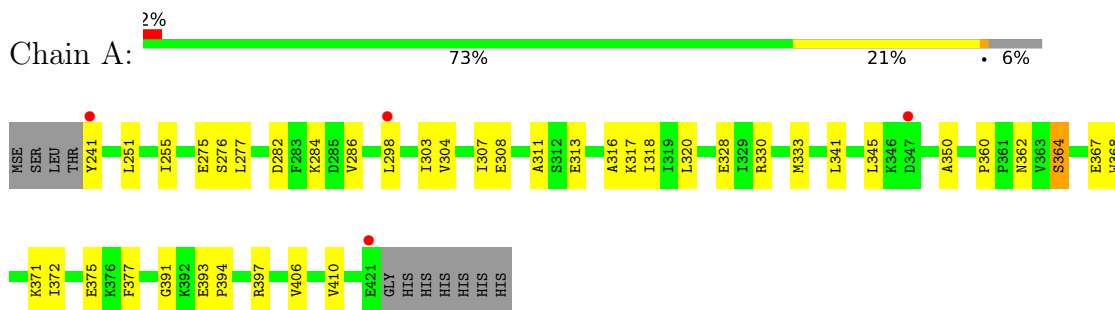
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total 90	O 90	0	0
3	B	91	Total 91	O 91	0	0
3	D	57	Total 57	O 57	0	0
3	E	92	Total 92	O 92	0	0

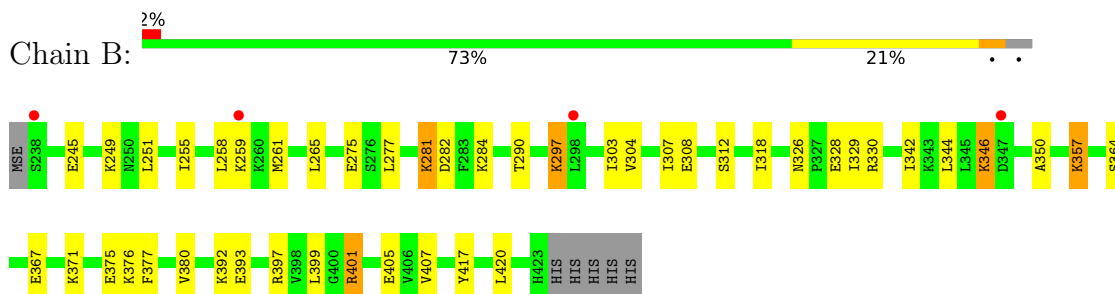
3 Residue-property plots [i](#)

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.

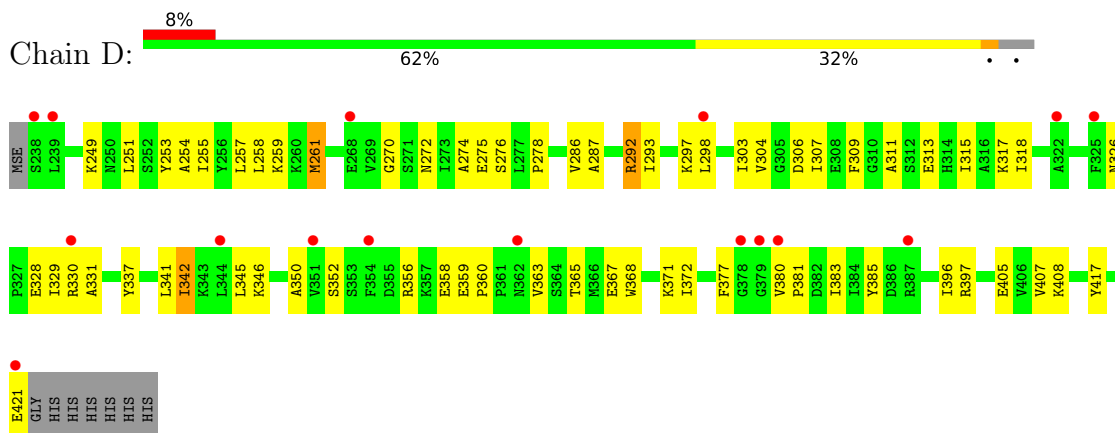
- Molecule 1: Uncharacterized protein MJ0236



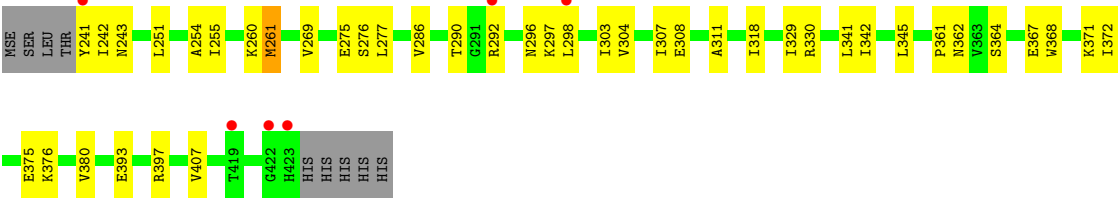
- Molecule 1: Uncharacterized protein MJ0236



- Molecule 1: Uncharacterized protein MJ0236



- Molecule 1: Uncharacterized protein MJ0236



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.08Å 112.14Å 67.25Å 90.00° 109.28° 90.00°	Depositor
Resolution (Å)	50.00 – 2.03 50.00 – 2.04	Depositor EDS
% Data completeness (in resolution range)	89.6 (50.00-2.03) 90.4 (50.00-2.04)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.03Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.238 0.217 , 0.239	Depositor DCC
R_{free} test set	2397 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6109	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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

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

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	0.42	0/1445	0.90	2/1935 (0.1%)
1	B	0.42	0/1485	0.88	4/1989 (0.2%)
1	D	0.39	0/1466	0.94	2/1964 (0.1%)
1	E	0.40	0/1464	0.87	4/1960 (0.2%)
All	All	0.41	0/5860	0.90	12/7848 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	304	VAL	N-CA-C	7.06	118.45	108.36
1	E	304	VAL	N-CA-C	6.97	118.32	108.36
1	A	304	VAL	N-CA-C	6.91	118.24	108.36
1	B	304	VAL	N-CA-C	6.76	117.64	108.17
1	E	277	LEU	N-CA-C	-6.04	101.33	110.39
1	B	312	SER	N-CA-C	5.98	119.71	107.69
1	B	277	LEU	N-CA-C	-5.84	101.63	110.39
1	D	261	MSE	N-CA-C	5.25	117.46	110.53
1	A	277	LEU	N-CA-C	-5.17	102.64	110.39
1	E	261	MSE	N-CA-C	5.13	118.07	110.48
1	E	296	ASN	N-CA-C	-5.04	98.39	107.75
1	B	290	THR	N-CA-C	-5.03	106.65	112.89

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	1423	0	1483	26	0
1	B	1462	0	1520	38	0
1	D	1444	0	1506	50	0
1	E	1441	0	1497	25	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
3	A	90	0	0	2	0
3	B	91	0	0	0	0
3	D	57	0	0	5	0
3	E	92	0	0	1	0
All	All	6109	0	6006	128	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 (128) 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:241:TYR:HB3	3:A:485:HOH:O	1.50	1.10
1:D:259:LYS:HG2	1:D:303:ILE:HD12	1.55	0.86
1:B:401:ARG:HH11	1:B:401:ARG:HG3	1.48	0.78
1:B:281:LYS:HA	1:B:281:LYS:HE2	1.70	0.74
1:B:401:ARG:HG3	1:B:401:ARG:NH1	2.01	0.73
1:D:329:ILE:HG13	1:D:380:VAL:HG11	1.70	0.72
1:B:401:ARG:NH1	1:B:405:GLU:OE2	2.22	0.72
1:D:318:ILE:HD13	1:D:397:ARG:HD3	1.71	0.72
1:D:255:ILE:HG22	1:D:259:LYS:HE3	1.71	0.71
1:D:297:LYS:HG3	1:E:311:ALA:O	1.92	0.70
1:D:259:LYS:HG2	1:D:303:ILE:CD1	2.20	0.70
1:B:261:MSE:HE1	1:B:407:VAL:HG13	1.75	0.69
1:B:344:LEU:HD11	1:B:420:LEU:HD21	1.74	0.68
1:E:261:MSE:HE1	1:E:407:VAL:HG12	1.76	0.68
1:D:421:GLU:HA	3:D:473:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:MSE:HE3	1:A:410:VAL:HG21	1.76	0.66
1:B:318:ILE:HD13	1:B:397:ARG:HD3	1.77	0.66
1:D:408:LYS:HE3	3:D:462:HOH:O	1.97	0.64
1:B:261:MSE:HE1	1:B:407:VAL:CG1	2.26	0.64
1:E:318:ILE:HD13	1:E:397:ARG:HD3	1.81	0.62
1:A:307:ILE:O	1:A:308:GLU:HG2	1.99	0.62
1:D:255:ILE:O	1:D:259:LYS:HG3	1.98	0.62
1:A:371:LYS:O	1:A:375:GLU:HG3	1.99	0.62
1:D:311:ALA:O	1:E:297:LYS:HD2	2.00	0.61
1:E:261:MSE:HE1	1:E:407:VAL:CG1	2.31	0.61
1:D:318:ILE:CD1	1:D:397:ARG:HD3	2.31	0.61
1:D:350:ALA:O	1:D:381:PRO:HB2	2.01	0.60
1:A:318:ILE:HD13	1:A:397:ARG:HD3	1.84	0.60
1:D:251:LEU:HB3	1:D:307:ILE:HD13	1.82	0.60
1:B:265:LEU:HD21	1:B:417:TYR:CG	2.37	0.60
1:B:259:LYS:HB3	1:B:259:LYS:NZ	2.18	0.59
1:E:241:TYR:O	1:E:242:ILE:HD13	2.03	0.59
1:D:261:MSE:HE1	1:D:407:VAL:CG1	2.33	0.59
1:E:269:VAL:HG13	1:E:393:GLU:OE1	2.04	0.58
1:B:259:LYS:HE3	1:D:306:ASP:OD1	2.04	0.57
1:E:255:ILE:HG23	1:E:303:ILE:HD13	1.85	0.57
1:B:401:ARG:HH11	1:B:401:ARG:CG	2.17	0.57
1:D:278:PRO:HG3	3:D:463:HOH:O	2.04	0.57
1:B:357:LYS:HB2	1:B:357:LYS:NZ	2.19	0.57
1:A:333:MSE:CE	1:A:406:VAL:HG12	2.35	0.56
1:B:344:LEU:CD1	1:B:420:LEU:HD21	2.34	0.56
1:D:261:MSE:HE1	1:D:407:VAL:HG13	1.88	0.56
1:D:258:LEU:HD21	1:D:293:ILE:HD13	1.88	0.55
1:D:368:TRP:CE2	1:D:372:ILE:HG13	2.43	0.54
1:A:251:LEU:O	1:A:255:ILE:HG12	2.08	0.53
1:A:255:ILE:HG23	1:A:303:ILE:HD13	1.89	0.53
1:B:342:ILE:CG2	1:B:346:LYS:HE3	2.38	0.53
1:D:275:GLU:HA	1:D:330:ARG:O	2.08	0.53
1:E:241:TYR:HE2	1:E:243:ASN:HD22	1.56	0.53
1:B:251:LEU:HB3	1:B:307:ILE:HD13	1.89	0.53
1:A:368:TRP:O	1:A:372:ILE:HG12	2.09	0.53
1:B:282:ASP:OD1	1:B:284:LYS:HB2	2.09	0.52
1:D:276:SER:HB3	1:D:286:VAL:HG22	1.91	0.52
1:D:287:ALA:HA	1:D:309:PHE:HA	1.91	0.52
1:D:345:LEU:HD13	1:D:383:ILE:CD1	2.40	0.52
1:E:364:SER:HB3	1:E:367:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ALA:HB1	1:B:377:PHE:CZ	2.46	0.50
1:B:259:LYS:HB3	1:B:259:LYS:HZ3	1.77	0.50
1:B:259:LYS:HE3	1:D:306:ASP:CG	2.37	0.50
1:D:337:TYR:HA	1:D:396:ILE:HG13	1.94	0.50
1:E:251:LEU:O	1:E:255:ILE:HG12	2.11	0.49
1:E:276:SER:HB3	1:E:286:VAL:HG22	1.93	0.49
1:B:371:LYS:O	1:B:375:GLU:HG3	2.13	0.49
1:D:272:ASN:ND2	1:E:297:LYS:NZ	2.60	0.49
1:A:391:GLY:HA2	1:B:392:LYS:O	2.12	0.49
1:D:345:LEU:HD13	1:D:383:ILE:HD13	1.94	0.49
1:D:360:PRO:O	1:D:363:VAL:HG22	2.12	0.49
1:A:307:ILE:C	1:A:308:GLU:HG2	2.39	0.48
1:A:311:ALA:O	1:B:297:LYS:HG2	2.13	0.48
1:B:307:ILE:C	1:B:308:GLU:HG2	2.39	0.47
1:B:364:SER:OG	1:B:367:GLU:HG3	2.14	0.47
1:B:329:ILE:HG13	1:B:380:VAL:HG11	1.95	0.47
1:D:385:TYR:C	1:D:385:TYR:CD1	2.92	0.47
1:B:307:ILE:O	1:B:308:GLU:HG2	2.14	0.47
1:D:254:ALA:HB1	1:D:407:VAL:HG21	1.97	0.47
1:A:333:MSE:CE	1:A:410:VAL:HG21	2.45	0.47
1:A:316:ALA:O	1:A:320:LEU:HD13	2.15	0.47
1:D:356:ARG:NH1	1:D:365:THR:HG21	2.30	0.47
1:A:364:SER:OG	1:A:367:GLU:HG3	2.14	0.47
1:B:326:ASN:OD1	1:B:328:GLU:HB2	2.15	0.47
1:E:260:LYS:HE2	3:E:472:HOH:O	2.15	0.47
1:E:329:ILE:HG13	1:E:380:VAL:HG11	1.96	0.46
1:D:275:GLU:HG3	1:D:331:ALA:HB2	1.97	0.46
1:B:399:LEU:HD12	1:B:399:LEU:N	2.30	0.46
1:A:360:PRO:HD2	1:A:368:TRP:CE2	2.50	0.46
1:B:255:ILE:HG23	1:B:303:ILE:HD13	1.98	0.45
1:A:350:ALA:HB1	1:A:377:PHE:CZ	2.51	0.45
1:A:282:ASP:OD1	1:A:284:LYS:HB2	2.16	0.45
1:E:361:PRO:O	1:E:362:ASN:HB2	2.16	0.45
1:E:341:LEU:O	1:E:345:LEU:HG	2.16	0.45
1:A:333:MSE:HE2	1:A:406:VAL:HG12	1.97	0.45
1:B:275:GLU:HA	1:B:330:ARG:O	2.16	0.45
1:B:259:LYS:CG	1:B:303:ILE:HD12	2.47	0.45
1:D:342:ILE:O	1:D:346:LYS:HG3	2.17	0.45
1:A:313:GLU:O	1:A:317:LYS:HG3	2.17	0.45
1:D:258:LEU:CD2	1:D:293:ILE:HD13	2.47	0.44
1:A:241:TYR:N	3:A:496:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:ASN:OD1	1:D:328:GLU:HB2	2.16	0.44
1:B:259:LYS:HG2	1:B:303:ILE:HD12	1.99	0.44
1:D:358:GLU:O	1:D:359:GLU:C	2.60	0.44
1:E:307:ILE:O	1:E:308:GLU:HG2	2.18	0.44
1:D:274:ALA:HB3	1:D:315:ILE:HG21	1.99	0.44
1:D:297:LYS:NZ	3:D:476:HOH:O	2.50	0.43
1:B:342:ILE:HG22	1:B:346:LYS:HE3	1.99	0.43
1:B:249:LYS:HD3	1:D:249:LYS:HB3	1.99	0.43
1:D:297:LYS:HG2	1:E:290:THR:O	2.19	0.43
1:E:275:GLU:HA	1:E:330:ARG:O	2.18	0.43
1:E:254:ALA:HB1	1:E:407:VAL:HG21	2.01	0.42
1:B:251:LEU:O	1:B:255:ILE:HG12	2.19	0.42
1:D:270:GLY:O	1:D:292:ARG:NH1	2.53	0.42
1:E:371:LYS:O	1:E:375:GLU:HG3	2.19	0.42
1:D:313:GLU:O	1:D:317:LYS:HG3	2.19	0.42
1:D:367:GLU:O	1:D:371:LYS:HG3	2.19	0.42
1:A:341:LEU:O	1:A:345:LEU:HG	2.19	0.42
1:A:308:GLU:OE1	1:E:260:LYS:NZ	2.52	0.41
1:D:255:ILE:CG2	1:D:259:LYS:HE3	2.47	0.41
1:B:245:GLU:HG3	1:D:253:TYR:CZ	2.56	0.41
1:D:330:ARG:HD3	3:D:463:HOH:O	2.19	0.41
1:D:341:LEU:HD22	1:D:417:TYR:CD1	2.55	0.41
1:D:352:SER:HB2	1:D:377:PHE:HB2	2.02	0.41
1:A:275:GLU:HA	1:A:330:ARG:O	2.20	0.41
1:A:393:GLU:HG2	1:A:394:PRO:O	2.21	0.41
1:E:376:LYS:HE3	1:E:376:LYS:HB2	1.87	0.41
1:A:276:SER:HB3	1:A:286:VAL:HG22	2.03	0.41
1:E:368:TRP:O	1:E:372:ILE:HG12	2.21	0.40
1:B:318:ILE:CD1	1:B:397:ARG:HD3	2.48	0.40
1:D:253:TYR:CE2	1:D:257:LEU:HD11	2.57	0.40
1:D:255:ILE:HG23	1:D:303:ILE:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	179/192 (93%)	175 (98%)	4 (2%)	0	100	100
1	B	184/192 (96%)	180 (98%)	3 (2%)	1 (0%)	24	17
1	D	182/192 (95%)	172 (94%)	10 (6%)	0	100	100
1	E	181/192 (94%)	176 (97%)	5 (3%)	0	100	100
All	All	726/768 (94%)	703 (97%)	22 (3%)	1 (0%)	48	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	346	LYS

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	154/160 (96%)	150 (97%)	4 (3%)	40	38
1	B	159/160 (99%)	152 (96%)	7 (4%)	25	18
1	D	157/160 (98%)	153 (98%)	4 (2%)	42	40
1	E	156/160 (98%)	153 (98%)	3 (2%)	50	50
All	All	626/640 (98%)	608 (97%)	18 (3%)	37	34

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	LEU
1	A	328	GLU
1	A	362	ASN
1	A	364	SER
1	B	258	LEU
1	B	281	LYS
1	B	297	LYS

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Mol	Chain	Res	Type
1	B	357	LYS
1	B	376	LYS
1	B	393	GLU
1	B	401	ARG
1	D	292	ARG
1	D	298	LEU
1	D	342	ILE
1	D	405	GLU
1	E	292	ARG
1	E	298	LEU
1	E	342	ILE

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	362	ASN
1	D	414	GLN
1	E	362	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	177/192 (92%)	0.11	4 (2%) 61 61	22, 34, 50, 58	0
1	B	182/192 (94%)	0.13	4 (2%) 62 62	22, 36, 50, 60	0
1	D	180/192 (93%)	0.81	16 (8%) 15 14	27, 46, 57, 63	0
1	E	179/192 (93%)	0.34	6 (3%) 48 47	24, 38, 54, 60	0
All	All	718/768 (93%)	0.35	30 (4%) 40 40	22, 38, 55, 63	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	TYR	4.8
1	E	422	GLY	3.3
1	E	423	HIS	3.3
1	D	238	SER	3.1
1	D	325	PHE	3.0
1	D	351	VAL	3.0
1	D	378	GLY	2.9
1	E	241	TYR	2.8
1	A	298	LEU	2.8
1	D	379	GLY	2.7
1	E	419	THR	2.5
1	D	421	GLU	2.5
1	D	322	ALA	2.4
1	B	259	LYS	2.4
1	D	387	ARG	2.4
1	D	362	ASN	2.3
1	B	298	LEU	2.3
1	D	239	LEU	2.3
1	E	298	LEU	2.3
1	B	347	ASP	2.3
1	D	298	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	344	LEU	2.3
1	D	330	ARG	2.2
1	B	238	SER	2.2
1	A	347	ASP	2.2
1	D	354	PHE	2.1
1	A	421	GLU	2.0
1	D	268	GLU	2.0
1	D	380	VAL	2.0
1	E	292	ARG	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	E	7	1/1	0.90	0.12	64,64,64,64	0
2	CL	A	6	1/1	0.92	0.14	49,49,49,49	0
2	CL	B	5	1/1	0.96	0.07	50,50,50,50	0
2	CL	E	3	1/1	0.96	0.08	48,48,48,48	0
2	CL	A	2	1/1	0.96	0.08	42,42,42,42	0
2	CL	D	4	1/1	0.97	0.08	54,54,54,54	0
2	CL	A	8	1/1	0.97	0.10	48,48,48,48	0
2	CL	B	9	1/1	0.97	0.07	46,46,46,46	0
2	CL	B	1	1/1	0.98	0.06	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.