



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:53 AM UTC

PDB ID : 4P22 / pdb_00004p22
Title : Crystal Structure of N-terminal Fragments of E1
Authors : Xie, S.-T.
Deposited on : 2014-02-28
Resolution : 2.75 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

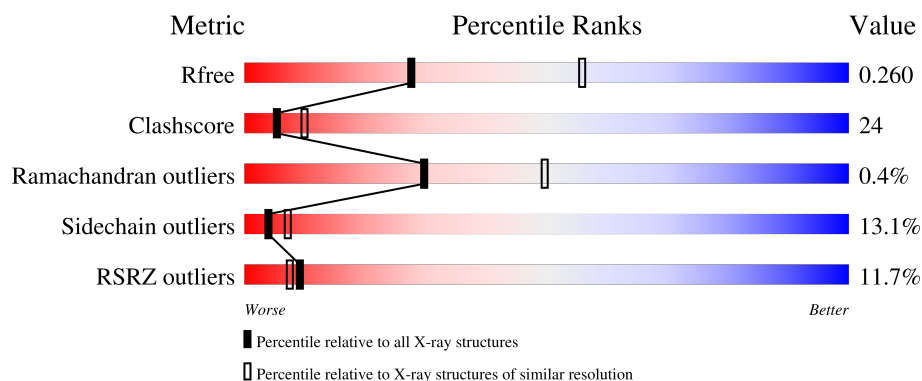
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	446	11% 50% 28% 5% 17%
1	B	446	8% 56% 22% 6% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5848 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 Ubiquitin-like modifier-activating enzyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2851	1812	487	537	15			
1	B	375	Total	C	N	O	S	0	0	0
			2888	1834	492	546	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP P22314
A	-5	PRO	-	expression tag	UNP P22314
A	-4	HIS	-	expression tag	UNP P22314
A	-3	MET	-	expression tag	UNP P22314
A	-2	ALA	-	expression tag	UNP P22314
A	-1	ASP	-	expression tag	UNP P22314
A	0	LEU	-	expression tag	UNP P22314
A	352	ASP	GLU	engineered mutation	UNP P22314
B	-6	GLY	-	expression tag	UNP P22314
B	-5	PRO	-	expression tag	UNP P22314
B	-4	HIS	-	expression tag	UNP P22314
B	-3	MET	-	expression tag	UNP P22314
B	-2	ALA	-	expression tag	UNP P22314
B	-1	ASP	-	expression tag	UNP P22314
B	0	LEU	-	expression tag	UNP P22314
B	352	ASP	GLU	engineered mutation	UNP P22314

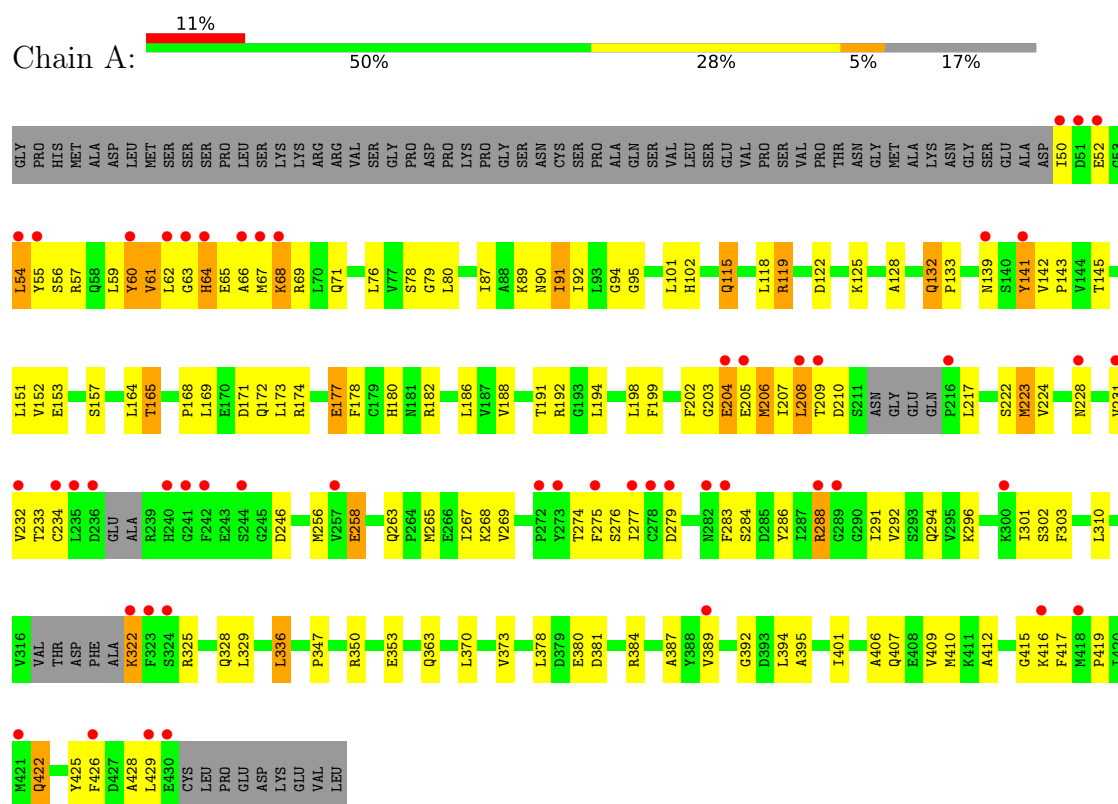
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	B	65	Total	O	0	0
			65	65		

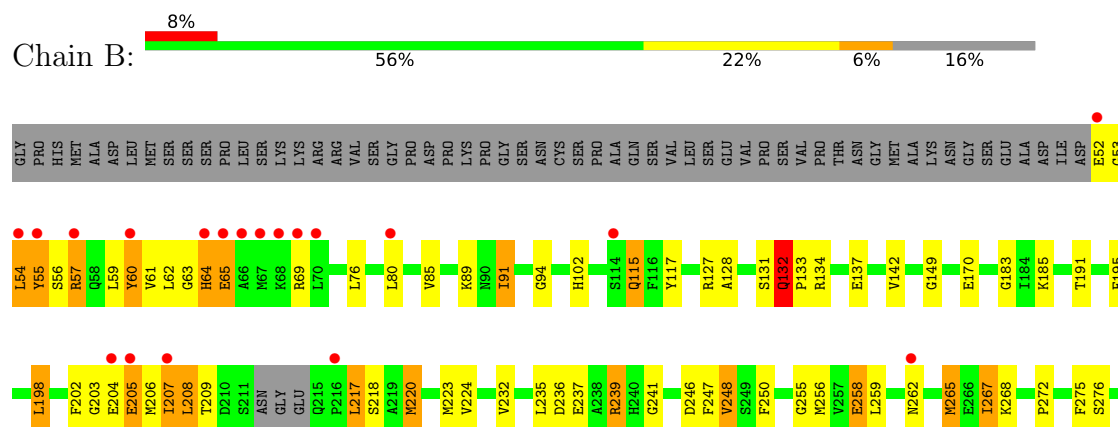
3 Residue-property plots [i](#)

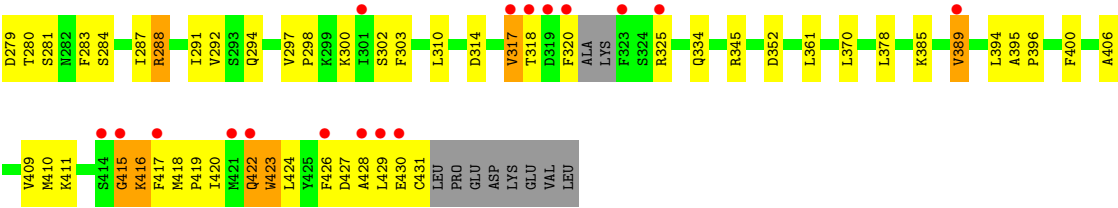
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ubiquitin-like modifier-activating enzyme 1



- Molecule 1: Ubiquitin-like modifier-activating enzyme 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	94.13Å 186.81Å 135.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.75 29.77 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.77-2.75) 98.3 (29.77-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.76Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.205 , 0.264 0.209 , 0.260	Depositor DCC
R_{free} test set	1559 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.0	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	0.92	EDS
Total number of atoms	5848	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 3.81% 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	0.55	0/2904	0.93	5/3929 (0.1%)
1	B	0.56	0/2943	0.98	8/3986 (0.2%)
All	All	0.56	0/5847	0.96	13/7915 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	THR	N-CA-C	-8.60	103.91	114.75
1	B	55	TYR	N-CA-C	7.51	119.47	111.28
1	B	416	LYS	N-CA-C	-7.22	104.05	112.92
1	A	141	TYR	N-CA-C	7.16	119.08	111.28
1	B	262	ASN	N-CA-C	6.47	119.08	110.53
1	A	288	ARG	N-CA-C	6.38	121.84	111.37
1	B	415	GLY	N-CA-C	6.02	121.42	110.95
1	B	142	VAL	N-CA-C	6.00	114.02	107.60
1	A	392	GLY	N-CA-C	5.84	119.48	111.54
1	A	60	TYR	N-CA-C	5.66	117.25	111.14
1	B	423	TRP	N-CA-C	5.65	118.45	109.24
1	A	373	VAL	CB-CA-C	-5.54	104.88	111.97
1	B	132	GLN	N-CA-C	5.39	120.08	112.75

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	2851	0	2835	139	0
1	B	2888	0	2860	174	0
2	A	44	0	0	0	0
2	B	65	0	0	4	0
All	All	5848	0	5695	275	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 24.

All (275) 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:B:80:LEU:CD2	1:B:128:ALA:HA	1.37	1.52
1:A:389:VAL:HG22	1:B:60:TYR:CE1	1.55	1.40
1:A:389:VAL:HG22	1:B:60:TYR:CZ	1.69	1.25
1:A:64:HIS:NE2	1:B:394:LEU:HA	1.57	1.19
1:B:80:LEU:HD22	1:B:128:ALA:CA	1.75	1.15
1:A:68:LYS:HD2	1:A:68:LYS:O	1.46	1.13
1:B:57:ARG:HA	1:B:60:TYR:CD2	1.89	1.07
1:B:207:ILE:HD11	1:B:416:LYS:HE3	1.25	1.07
1:B:422:GLN:HE21	1:B:422:GLN:CA	1.59	1.06
1:B:422:GLN:HA	1:B:422:GLN:NE2	1.58	1.06
1:B:80:LEU:CD2	1:B:128:ALA:CA	2.33	1.04
1:A:389:VAL:CG2	1:B:60:TYR:CE1	2.40	1.03
1:B:428:ALA:O	1:B:429:LEU:HD12	1.58	1.03
1:B:80:LEU:HD22	1:B:128:ALA:HA	1.03	1.00
1:B:422:GLN:HG3	2:B:524:HOH:O	1.57	1.00
1:B:207:ILE:CD1	1:B:416:LYS:HE3	1.92	0.98
1:B:80:LEU:HD23	1:B:128:ALA:HA	1.41	0.98
1:B:428:ALA:C	1:B:429:LEU:HD12	1.88	0.97
1:B:62:LEU:HD22	1:B:417:PHE:HD2	1.27	0.96
1:B:314:ASP:O	1:B:422:GLN:HB2	1.65	0.94
1:A:429:LEU:HD13	1:B:59:LEU:HD22	1.50	0.93
1:B:62:LEU:HD22	1:B:417:PHE:CD2	2.04	0.93
1:A:389:VAL:HG22	1:B:60:TYR:OH	1.68	0.91
1:A:91:ILE:HD11	1:A:409:VAL:HG11	1.49	0.91
1:B:57:ARG:HA	1:B:60:TYR:CE2	2.05	0.90
1:A:268:LYS:HB3	1:A:276:SER:OG	1.71	0.90
1:A:394:LEU:HA	1:B:64:HIS:NE2	1.86	0.88
1:B:422:GLN:HE21	1:B:422:GLN:HA	0.74	0.88
1:B:427:ASP:OD2	1:B:429:LEU:HD13	1.74	0.88
1:B:56:SER:O	1:B:60:TYR:CE1	2.27	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:HIS:HB2	1:B:94:GLY:O	1.74	0.88
1:A:389:VAL:HG22	1:B:60:TYR:HE1	1.29	0.86
1:A:52:GLU:HG2	1:A:279:ASP:OD1	1.77	0.84
1:A:80:LEU:HD11	1:A:101:LEU:HB3	1.60	0.82
1:A:389:VAL:CG2	1:B:60:TYR:OH	2.28	0.82
1:A:60:TYR:OH	1:B:389:VAL:HG22	1.81	0.80
1:A:199:PHE:HA	1:A:422:GLN:O	1.80	0.80
1:B:62:LEU:CD2	1:B:417:PHE:HD2	1.94	0.80
1:A:68:LYS:O	1:A:68:LYS:CD	2.30	0.79
1:B:63:GLY:O	1:B:64:HIS:CD2	2.35	0.79
1:A:389:VAL:CG2	1:B:60:TYR:HE1	1.84	0.78
1:A:64:HIS:CD2	1:B:394:LEU:HA	2.19	0.78
1:B:59:LEU:HD23	1:B:417:PHE:CZ	2.20	0.77
1:A:429:LEU:CD1	1:B:59:LEU:HD22	2.15	0.76
1:B:94:GLY:HA3	1:B:410:MET:HE1	1.67	0.75
1:A:381:ASP:OD1	1:A:384:ARG:NH2	2.21	0.74
1:B:202:PHE:HB3	1:B:206:MET:HE3	1.69	0.74
1:B:63:GLY:O	1:B:64:HIS:CB	2.35	0.74
1:B:63:GLY:O	1:B:64:HIS:HB3	1.87	0.73
1:B:56:SER:C	1:B:60:TYR:CZ	2.67	0.73
1:B:258:GLU:HG3	1:B:283:PHE:CG	2.24	0.72
1:A:122:ASP:HA	1:A:125:LYS:HD2	1.72	0.72
1:A:64:HIS:HB2	1:A:94:GLY:HA2	1.72	0.71
1:A:303:PHE:HZ	1:A:419:PRO:HG2	1.54	0.71
1:A:363:GLN:NE2	1:A:380:GLU:OE2	2.24	0.70
1:B:430:GLU:C	1:B:430:GLU:OE1	2.35	0.70
1:B:207:ILE:HB	1:B:300:LYS:HE3	1.73	0.70
1:B:80:LEU:HD22	1:B:128:ALA:CB	2.22	0.70
1:B:246:ASP:OD2	1:B:294:GLN:NE2	2.25	0.69
1:B:61:VAL:HG13	1:B:69:ARG:HD2	1.73	0.69
1:B:56:SER:O	1:B:60:TYR:CZ	2.46	0.69
1:B:422:GLN:CA	1:B:422:GLN:NE2	2.30	0.68
1:B:56:SER:O	1:B:60:TYR:CD1	2.46	0.68
1:A:429:LEU:HD13	1:B:59:LEU:CD2	2.21	0.67
1:A:60:TYR:CZ	1:B:389:VAL:HG22	2.29	0.67
1:A:132:GLN:HG3	1:A:133:PRO:HD3	1.77	0.66
1:A:63:GLY:O	1:A:64:HIS:CD2	2.48	0.66
1:B:62:LEU:CD2	1:B:417:PHE:CD2	2.75	0.66
1:A:325:ARG:HG3	1:A:328:GLN:HG3	1.78	0.66
1:A:60:TYR:CE2	1:B:389:VAL:HA	2.30	0.65
1:A:246:ASP:OD2	1:A:294:GLN:NE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:ASP:OD2	1:B:428:ALA:N	2.30	0.65
1:A:395:ALA:N	1:B:64:HIS:NE2	2.45	0.64
1:B:204:GLU:HA	1:B:302:SER:HA	1.80	0.64
1:B:57:ARG:CA	1:B:60:TYR:CE2	2.81	0.63
1:A:63:GLY:O	1:A:64:HIS:HD2	1.81	0.63
1:A:139:ASN:HB2	1:A:141:TYR:CE1	2.35	0.62
1:B:117:TYR:CE2	1:B:134:ARG:HB3	2.35	0.62
1:B:85:VAL:HG11	1:B:115:GLN:HA	1.80	0.62
1:B:279:ASP:C	1:B:279:ASP:OD2	2.43	0.61
1:A:325:ARG:HG2	1:A:328:GLN:HE21	1.66	0.61
1:B:208:LEU:HA	1:B:416:LYS:O	2.01	0.61
1:B:63:GLY:O	1:B:64:HIS:CG	2.54	0.60
1:B:64:HIS:CG	1:B:94:GLY:HA2	2.36	0.60
1:B:115:GLN:C	1:B:115:GLN:OE1	2.45	0.60
1:B:207:ILE:HD11	1:B:416:LYS:CE	2.17	0.59
1:B:411:LYS:O	1:B:415:GLY:N	2.35	0.59
1:B:56:SER:HB3	1:B:60:TYR:OH	2.02	0.58
1:B:411:LYS:NZ	2:B:545:HOH:O	2.32	0.58
1:A:275:PHE:HE1	1:A:277:ILE:CG2	2.15	0.58
1:B:63:GLY:O	1:B:64:HIS:HD2	1.83	0.57
1:B:303:PHE:HZ	1:B:419:PRO:HG2	1.69	0.57
1:A:64:HIS:HB2	1:A:94:GLY:CA	2.33	0.57
1:B:198:LEU:HD12	1:B:420:ILE:HD12	1.86	0.57
1:A:60:TYR:HE2	1:B:389:VAL:HA	1.69	0.57
1:A:68:LYS:HD2	1:A:68:LYS:C	2.26	0.57
1:B:258:GLU:HG3	1:B:283:PHE:CD2	2.40	0.56
1:A:62:LEU:HD12	1:A:415:GLY:HA3	1.87	0.56
1:A:153:GLU:HB2	1:A:178:PHE:CE1	2.40	0.56
1:A:350:ARG:HG3	1:B:57:ARG:HD3	1.87	0.55
1:A:60:TYR:OH	1:B:389:VAL:CG2	2.53	0.55
1:B:303:PHE:CZ	1:B:419:PRO:HG2	2.42	0.55
1:A:233:THR:HG22	1:A:274:THR:HG22	1.89	0.55
1:A:60:TYR:OH	1:B:389:VAL:HG13	2.07	0.54
1:A:268:LYS:HB3	1:A:276:SER:HG	1.72	0.54
1:B:420:ILE:HG22	1:B:422:GLN:O	2.07	0.54
1:A:64:HIS:NE2	1:B:394:LEU:CA	2.50	0.54
1:A:204:GLU:HA	1:A:303:PHE:H	1.73	0.54
1:A:394:LEU:CA	1:B:64:HIS:NE2	2.66	0.54
1:B:91:ILE:HD12	1:B:410:MET:HE2	1.90	0.53
1:B:64:HIS:HB2	1:B:94:GLY:C	2.32	0.53
1:A:169:LEU:O	1:A:173:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:NH2	1:B:53:GLY:HA2	2.23	0.53
1:A:192:ARG:HD3	1:A:336:LEU:HD23	1.90	0.53
1:B:385:LYS:O	1:B:389:VAL:HB	2.08	0.53
1:B:62:LEU:HD11	1:B:411:LYS:HA	1.91	0.53
1:A:50:ILE:HG22	1:A:52:GLU:H	1.73	0.53
1:B:64:HIS:CB	1:B:94:GLY:HA2	2.38	0.53
1:A:115:GLN:CD	1:A:118:LEU:HD13	2.34	0.52
1:A:322:LYS:HD3	1:B:317:VAL:HG22	1.91	0.52
1:B:115:GLN:NE2	1:B:131:SER:OG	2.42	0.52
1:A:171:ASP:OD2	1:A:174:ARG:NH2	2.43	0.52
1:A:207:ILE:O	1:A:416:LYS:HB3	2.08	0.52
1:B:279:ASP:OD2	1:B:280:THR:N	2.42	0.52
1:A:407:GLN:HG2	1:B:396:PRO:HB2	1.92	0.52
1:B:115:GLN:OE1	1:B:115:GLN:CA	2.57	0.52
1:B:207:ILE:HG13	1:B:300:LYS:HZ2	1.73	0.52
1:A:286:TYR:OH	1:A:288:ARG:O	2.25	0.52
1:B:207:ILE:CD1	1:B:416:LYS:CE	2.78	0.52
1:B:287:ILE:HG22	1:B:288:ARG:HD2	1.91	0.52
1:B:411:LYS:O	1:B:415:GLY:HA3	2.09	0.52
1:A:258:GLU:HG3	1:A:283:PHE:CD2	2.45	0.52
1:A:223:MET:HA	1:A:286:TYR:CE2	2.45	0.52
1:B:132:GLN:HG3	1:B:133:PRO:HD3	1.90	0.52
1:B:267:ILE:HG13	1:B:275:PHE:CD1	2.45	0.52
1:B:64:HIS:HB2	1:B:94:GLY:HA2	1.92	0.51
1:A:199:PHE:CE1	1:A:422:GLN:HB3	2.45	0.51
1:A:164:LEU:HB2	1:A:188:VAL:HG22	1.92	0.51
1:B:208:LEU:HD13	1:B:418:MET:HG2	1.91	0.51
1:A:303:PHE:CZ	1:A:419:PRO:HG2	2.42	0.51
1:B:279:ASP:OD2	1:B:281:SER:OG	2.28	0.51
1:B:422:GLN:HB3	1:B:423:TRP:CD1	2.46	0.51
1:B:256:MET:HG3	1:B:283:PHE:HB3	1.92	0.50
1:B:314:ASP:HB2	1:B:422:GLN:HG2	1.93	0.50
1:A:64:HIS:CD2	1:B:394:LEU:CA	2.94	0.50
1:A:256:MET:HB3	1:A:284:SER:O	2.11	0.50
1:A:279:ASP:O	1:A:279:ASP:OD2	2.30	0.50
1:A:208:LEU:HD23	1:A:301:ILE:HB	1.94	0.50
1:B:195:PHE:CD1	1:B:389:VAL:HG11	2.46	0.50
1:A:60:TYR:OH	1:B:389:VAL:CB	2.59	0.50
1:B:423:TRP:CD1	1:B:423:TRP:N	2.79	0.50
1:B:426:PHE:CZ	1:B:428:ALA:HA	2.47	0.49
1:A:194:LEU:HD13	1:A:389:VAL:CG1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:H	1:A:217:LEU:HD23	1.78	0.49
1:A:417:PHE:O	1:A:419:PRO:HD3	2.12	0.49
1:A:329:LEU:HD12	1:A:425:TYR:HB3	1.94	0.49
1:B:59:LEU:HD23	1:B:417:PHE:CE1	2.48	0.49
1:A:419:PRO:O	1:B:430:GLU:OE2	2.30	0.49
1:B:220:MET:HE3	1:B:291:ILE:HG12	1.95	0.49
1:B:280:THR:HG22	1:B:283:PHE:CD1	2.48	0.49
1:B:224:VAL:HG22	1:B:232:VAL:HG22	1.95	0.48
1:A:54:LEU:HB3	1:A:263:GLN:HB2	1.95	0.48
1:B:422:GLN:HB3	1:B:423:TRP:HD1	1.78	0.48
1:B:248:VAL:HG13	1:B:292:VAL:HG23	1.95	0.48
1:B:60:TYR:O	1:B:65:GLU:HB3	2.13	0.48
1:B:185:LYS:NZ	1:B:206:MET:HE1	2.29	0.48
1:B:239:ARG:HD2	1:B:272:PRO:O	2.12	0.48
1:B:411:LYS:O	1:B:415:GLY:CA	2.62	0.48
1:A:222:SER:HB2	1:A:234:CYS:HA	1.96	0.48
1:A:389:VAL:CG2	1:B:60:TYR:CZ	2.64	0.48
1:A:203:GLY:C	1:A:205:GLU:H	2.22	0.48
1:B:80:LEU:HD23	1:B:131:SER:HB2	1.96	0.47
1:A:80:LEU:CD1	1:A:101:LEU:HB3	2.37	0.47
1:A:325:ARG:CG	1:A:328:GLN:HG3	2.43	0.47
1:B:132:GLN:HG3	1:B:133:PRO:CD	2.44	0.47
1:B:208:LEU:CA	1:B:416:LYS:O	2.62	0.47
1:A:56:SER:HA	1:A:59:LEU:HD12	1.96	0.47
1:B:64:HIS:HB2	1:B:94:GLY:CA	2.44	0.47
1:A:60:TYR:OH	1:B:389:VAL:CA	2.62	0.47
1:A:199:PHE:CD1	1:A:422:GLN:O	2.68	0.47
1:B:57:ARG:N	1:B:60:TYR:CE2	2.82	0.46
1:A:92:ILE:O	1:A:139:ASN:ND2	2.48	0.46
1:B:427:ASP:OD2	1:B:427:ASP:C	2.57	0.46
1:A:55:TYR:CE1	1:A:417:PHE:HE1	2.33	0.46
1:A:87:ILE:O	1:A:91:ILE:HB	2.16	0.46
1:B:430:GLU:OE1	1:B:430:GLU:O	2.32	0.46
1:B:56:SER:CB	1:B:60:TYR:OH	2.63	0.46
1:A:80:LEU:HD13	1:A:128:ALA:HA	1.98	0.46
1:A:192:ARG:HD3	1:A:336:LEU:CD2	2.46	0.46
1:B:203:GLY:C	1:B:205:GLU:H	2.23	0.46
1:A:204:GLU:HG2	1:A:303:PHE:O	2.16	0.46
1:A:64:HIS:CB	1:A:94:GLY:HA2	2.43	0.46
1:B:56:SER:C	1:B:60:TYR:CE2	2.94	0.46
1:A:79:GLY:HA3	1:A:165:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:HD23	1:A:329:LEU:HA	1.69	0.45
1:B:428:ALA:C	1:B:429:LEU:CD1	2.75	0.45
1:A:64:HIS:HB2	1:A:94:GLY:O	2.16	0.45
1:A:78:SER:O	1:A:165:THR:HB	2.17	0.45
1:B:223:MET:HE3	1:B:223:MET:HB3	1.70	0.45
1:B:406:ALA:O	1:B:410:MET:HG2	2.16	0.45
1:A:61:VAL:HG22	1:A:66:ALA:HB3	1.98	0.45
1:A:275:PHE:CE1	1:A:277:ILE:CG2	2.98	0.45
1:A:389:VAL:HG23	1:B:60:TYR:OH	2.14	0.45
1:A:50:ILE:HG22	1:A:52:GLU:N	2.32	0.45
1:B:255:GLY:O	1:B:284:SER:HB2	2.16	0.45
1:A:61:VAL:HG11	1:A:69:ARG:NH2	2.32	0.45
1:A:60:TYR:O	1:A:65:GLU:HB3	2.17	0.44
1:A:89:LYS:HE3	1:A:90:ASN:OD1	2.16	0.44
1:A:203:GLY:O	1:A:205:GLU:N	2.49	0.44
1:B:59:LEU:CD2	1:B:417:PHE:CE1	3.00	0.44
1:B:280:THR:HG22	1:B:283:PHE:CE1	2.52	0.44
1:B:352:ASP:OD2	1:B:352:ASP:N	2.49	0.44
1:A:224:VAL:HG12	1:A:286:TYR:CD1	2.53	0.44
1:B:89:LYS:HE3	1:B:89:LYS:HB3	1.66	0.44
1:B:325:ARG:H	1:B:325:ARG:HG3	1.61	0.44
1:A:178:PHE:CZ	1:A:182:ARG:HD3	2.53	0.44
1:B:91:ILE:HD11	1:B:409:VAL:HB	1.99	0.44
1:A:64:HIS:HD2	1:B:394:LEU:HB3	1.82	0.44
1:A:94:GLY:HA3	1:A:410:MET:HE1	1.99	0.44
1:A:102:HIS:CG	1:A:151:LEU:HD21	2.53	0.44
1:A:141:TYR:CD2	1:A:142:VAL:HG23	2.52	0.44
1:A:206:MET:HE1	1:A:416:LYS:HG2	2.00	0.44
1:A:406:ALA:O	1:A:410:MET:HG2	2.18	0.44
1:B:102:HIS:NE2	1:B:149:GLY:O	2.48	0.44
1:B:69:ARG:HB2	2:B:543:HOH:O	2.17	0.43
1:A:322:LYS:HB3	1:A:322:LYS:HE2	1.80	0.43
1:A:60:TYR:HB3	1:A:65:GLU:HG2	1.99	0.43
1:B:60:TYR:CD1	1:B:60:TYR:N	2.84	0.43
1:B:54:LEU:H	1:B:54:LEU:HD22	1.82	0.43
1:B:268:LYS:HB3	1:B:276:SER:OG	2.18	0.43
1:A:202:PHE:CE2	1:A:419:PRO:HB3	2.54	0.43
1:A:232:VAL:HG21	1:A:275:PHE:CE1	2.54	0.43
1:A:206:MET:HE2	1:A:206:MET:HA	2.01	0.43
1:B:297:VAL:HA	1:B:298:PRO:HD3	1.86	0.43
1:A:69:ARG:O	1:A:71:GLN:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ARG:CG	1:A:328:GLN:HE21	2.31	0.43
1:B:80:LEU:HD23	1:B:127:ARG:O	2.18	0.43
1:A:57:ARG:HB2	1:A:263:GLN:HE22	1.83	0.42
1:A:64:HIS:NE2	1:B:395:ALA:N	2.66	0.42
1:A:153:GLU:HB2	1:A:178:PHE:CZ	2.54	0.42
1:A:178:PHE:CE1	1:A:182:ARG:HD3	2.54	0.42
1:B:207:ILE:HB	1:B:300:LYS:CE	2.46	0.42
1:A:54:LEU:HD22	1:A:265:MET:HG2	2.01	0.42
1:B:64:HIS:O	1:B:64:HIS:ND1	2.52	0.42
1:A:202:PHE:CZ	1:A:412:ALA:HB2	2.55	0.42
1:A:177:GLU:HG3	1:A:178:PHE:N	2.35	0.42
1:B:80:LEU:HD23	1:B:128:ALA:CA	2.29	0.42
1:B:195:PHE:HD1	1:B:389:VAL:HG11	1.84	0.42
1:A:119:ARG:HH12	1:B:137:GLU:HB3	1.85	0.42
1:B:55:TYR:HB2	1:B:247:PHE:CD2	2.54	0.42
1:B:426:PHE:CE1	1:B:427:ASP:O	2.73	0.42
1:A:95:GLY:HA2	1:A:142:VAL:HG21	2.02	0.42
1:A:426:PHE:CZ	1:A:428:ALA:HA	2.55	0.42
1:B:250:PHE:HE1	1:B:265:MET:HE1	1.85	0.41
1:A:62:LEU:CD1	1:A:415:GLY:HA3	2.49	0.41
1:B:94:GLY:HA3	1:B:410:MET:CE	2.44	0.41
1:A:419:PRO:C	1:B:430:GLU:OE2	2.64	0.41
1:A:232:VAL:HG23	1:A:277:ILE:HG23	2.02	0.41
1:B:258:GLU:CD	1:B:258:GLU:H	2.28	0.41
1:B:183:GLY:HA2	2:B:559:HOH:O	2.20	0.41
1:B:208:LEU:CB	1:B:416:LYS:O	2.69	0.41
1:A:142:VAL:HA	1:A:143:PRO:HD3	1.92	0.41
1:B:427:ASP:CG	1:B:429:LEU:HD13	2.43	0.41
1:A:63:GLY:O	1:B:394:LEU:HD22	2.20	0.41
1:A:168:PRO:O	1:A:172:GLN:HG3	2.21	0.40
1:A:61:VAL:CG1	1:A:69:ARG:NE	2.84	0.40
1:B:202:PHE:CE2	1:B:419:PRO:HB3	2.56	0.40
1:B:265:MET:HB2	1:B:265:MET:HE3	1.52	0.40
1:A:180:HIS:NE2	1:A:204:GLU:HG3	2.35	0.40
1:A:347:PRO:HB2	1:A:387:ALA:O	2.21	0.40
1:B:205:GLU:H	1:B:205:GLU:HG3	1.65	0.40
1:B:314:ASP:O	1:B:422:GLN:CB	2.53	0.40
1:A:350:ARG:CG	1:B:57:ARG:HD3	2.52	0.40
1:A:66:ALA:O	1:A:69:ARG:HD3	2.22	0.40
1:B:217:LEU:HD11	1:B:241:GLY:HA3	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	362/446 (81%)	341 (94%)	20 (6%)	1 (0%)	36	56
1	B	369/446 (83%)	352 (95%)	15 (4%)	2 (0%)	24	43
All	All	731/892 (82%)	693 (95%)	35 (5%)	3 (0%)	30	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	HIS
1	A	204	GLU
1	B	317	VAL

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	308/372 (83%)	268 (87%)	40 (13%)	4	7
1	B	312/372 (84%)	271 (87%)	41 (13%)	4	7
All	All	620/744 (83%)	539 (87%)	81 (13%)	4	7

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	61	VAL
1	A	64	HIS

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Mol	Chain	Res	Type
1	A	67	MET
1	A	68	LYS
1	A	76	LEU
1	A	91	ILE
1	A	115	GLN
1	A	119	ARG
1	A	132	GLN
1	A	145	THR
1	A	152	VAL
1	A	157	SER
1	A	165	THR
1	A	177	GLU
1	A	186	LEU
1	A	191	THR
1	A	198	LEU
1	A	206	MET
1	A	208	LEU
1	A	209	THR
1	A	210	ASP
1	A	223	MET
1	A	228	ASN
1	A	231	VAL
1	A	258	GLU
1	A	267	ILE
1	A	269	VAL
1	A	291	ILE
1	A	292	VAL
1	A	296	LYS
1	A	302	SER
1	A	310	LEU
1	A	322	LYS
1	A	336	LEU
1	A	353	GLU
1	A	370	LEU
1	A	378	LEU
1	A	401	ILE
1	A	422	GLN
1	B	52	GLU
1	B	54	LEU
1	B	57	ARG
1	B	60	TYR
1	B	65	GLU

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Mol	Chain	Res	Type
1	B	76	LEU
1	B	91	ILE
1	B	115	GLN
1	B	132	GLN
1	B	170	GLU
1	B	191	THR
1	B	198	LEU
1	B	205	GLU
1	B	207	ILE
1	B	208	LEU
1	B	209	THR
1	B	217	LEU
1	B	218	SER
1	B	220	MET
1	B	235	LEU
1	B	236	ASP
1	B	237	GLU
1	B	239	ARG
1	B	248	VAL
1	B	258	GLU
1	B	259	LEU
1	B	265	MET
1	B	267	ILE
1	B	288	ARG
1	B	310	LEU
1	B	320	PHE
1	B	334	GLN
1	B	345	ARG
1	B	361	LEU
1	B	370	LEU
1	B	378	LEU
1	B	389	VAL
1	B	400	PHE
1	B	422	GLN
1	B	424	LEU
1	B	431	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	197	GLN

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Mol	Chain	Res	Type
1	B	197	GLN
1	B	334	GLN
1	B	422	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 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	370/446 (82%)	0.46	51 (13%) 6 5	16, 41, 107, 152	0
1	B	375/446 (84%)	0.12	36 (9%) 13 13	15, 36, 78, 135	0
All	All	745/892 (83%)	0.29	87 (11%) 9 7	15, 38, 100, 152	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	TYR	9.1
1	A	235	LEU	6.2
1	A	66	ALA	6.1
1	A	54	LEU	5.9
1	B	205	GLU	5.9
1	B	317	VAL	5.9
1	B	415	GLY	5.8
1	B	204	GLU	5.6
1	A	50	ILE	5.6
1	B	323	PHE	5.5
1	A	279	ASP	5.5
1	B	70	LEU	5.4
1	A	257	VAL	5.2
1	A	204	GLU	5.0
1	B	54	LEU	4.8
1	B	67	MET	4.8
1	B	66	ALA	4.7
1	A	278	CYS	4.5
1	A	416	LYS	4.5
1	B	422	GLN	4.5
1	A	67	MET	4.5
1	B	52	GLU	4.4
1	A	55	TYR	4.4
1	A	242	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	64	HIS	4.3
1	B	64	HIS	4.3
1	A	60	TYR	4.3
1	A	51	ASP	4.0
1	A	240	HIS	4.0
1	B	430	GLU	4.0
1	A	216	PRO	4.0
1	B	320	PHE	4.0
1	B	429	LEU	3.9
1	A	63	GLY	3.8
1	A	323	PHE	3.8
1	B	414	SER	3.8
1	B	319	ASP	3.7
1	A	429	LEU	3.7
1	A	232	VAL	3.6
1	A	421	MET	3.6
1	A	231	VAL	3.4
1	B	318	THR	3.4
1	B	114	SER	3.3
1	A	139	ASN	3.3
1	B	68	LYS	3.1
1	A	209	THR	3.1
1	B	426	PHE	3.1
1	A	236	ASP	3.1
1	A	275	PHE	3.1
1	B	80	LEU	3.0
1	A	277	ILE	3.0
1	A	282	ASN	2.9
1	A	288	ARG	2.8
1	A	289	GLY	2.8
1	A	273	TYR	2.8
1	A	430	GLU	2.8
1	A	141	TYR	2.8
1	A	324	SER	2.7
1	B	301	ILE	2.6
1	B	421	MET	2.5
1	B	69	ARG	2.5
1	A	426	PHE	2.5
1	B	428	ALA	2.5
1	A	205	GLU	2.4
1	B	65	GLU	2.4
1	B	55	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	68	LYS	2.4
1	B	207	ILE	2.3
1	B	325	ARG	2.3
1	A	241	GLY	2.3
1	A	300	LYS	2.3
1	A	322	LYS	2.3
1	A	52	GLU	2.2
1	A	244	SER	2.2
1	A	208	LEU	2.2
1	B	417	PHE	2.2
1	A	234	CYS	2.2
1	A	228	ASN	2.2
1	A	418	MET	2.2
1	A	283	PHE	2.2
1	B	57	ARG	2.1
1	B	216	PRO	2.1
1	A	62	LEU	2.1
1	A	272	PRO	2.1
1	B	262	ASN	2.1
1	B	389	VAL	2.1
1	A	389	VAL	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.