



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:45 PM UTC

PDB ID : 3LFV / pdb_00003lfv
Title : crystal structure of unliganded PDE5A GAF domain
Authors : Wang, H.; Robinson, H.; Ke, H.
Deposited on : 2010-01-18
Resolution : 2.80 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

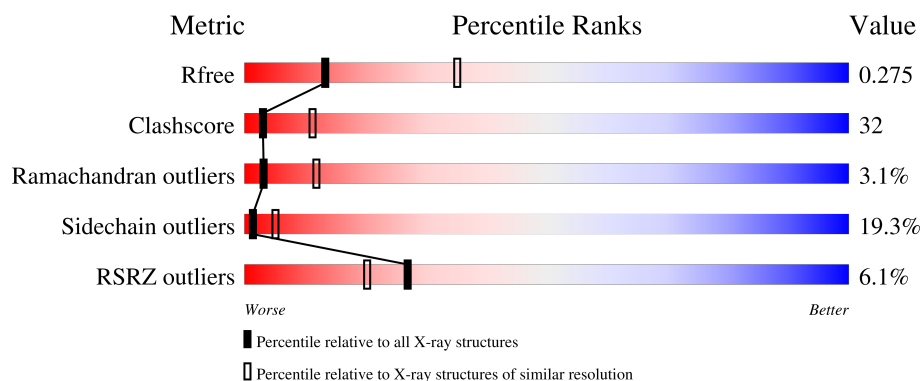
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	431	
1	B	431	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6110 atoms, of which 0 are hydrogens and 0 are deuteriums.

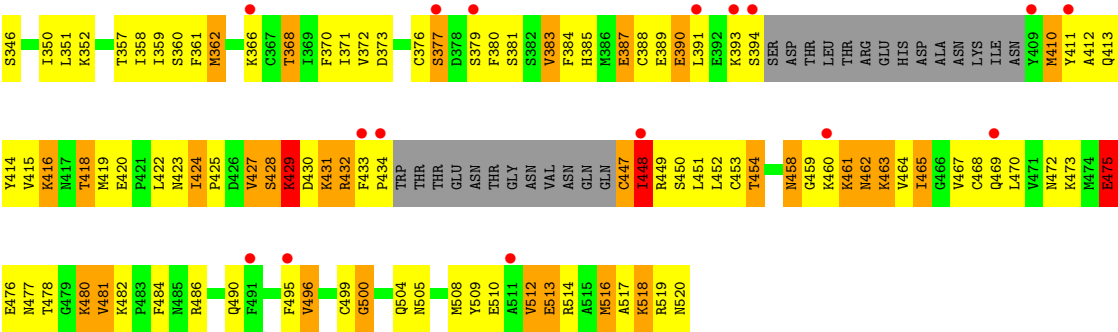
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called cGMP-specific 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3097	1955	524	595	23			
1	B	380	Total	C	N	O	S	0	0	0
			3013	1903	511	576	23			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	ALA	-	expression tag	UNP O76074
A	91	MET	-	expression tag	UNP O76074
A	92	GLU	-	expression tag	UNP O76074
A	93	HIS	-	expression tag	UNP O76074
A	94	MET	-	expression tag	UNP O76074
A	95	ALA	-	expression tag	UNP O76074
A	96	SER	-	expression tag	UNP O76074
A	97	MET	-	expression tag	UNP O76074
A	149	SER	CYS	engineered mutation	UNP O76074
A	519	ARG	-	expression tag	UNP O76074
A	520	ASN	-	expression tag	UNP O76074
B	90	ALA	-	expression tag	UNP O76074
B	91	MET	-	expression tag	UNP O76074
B	92	GLU	-	expression tag	UNP O76074
B	93	HIS	-	expression tag	UNP O76074
B	94	MET	-	expression tag	UNP O76074
B	95	ALA	-	expression tag	UNP O76074
B	96	SER	-	expression tag	UNP O76074
B	97	MET	-	expression tag	UNP O76074
B	149	SER	CYS	engineered mutation	UNP O76074
B	519	ARG	-	expression tag	UNP O76074
B	520	ASN	-	expression tag	UNP O76074



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.19Å 144.19Å 134.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.80) 99.7 (30.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.240 , 0.285 0.234 , 0.275	Depositor DCC
R_{free} test set	2236 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6110	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.39	0/3145	0.69	3/4232 (0.1%)
1	B	0.37	0/3058	0.66	0/4110
All	All	0.38	0/6203	0.67	3/8342 (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	15
1	B	0	12
All	All	0	27

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	LYS	N-CA-C	-5.37	107.73	114.56
1	A	269	MET	CA-C-N	5.17	124.93	119.76
1	A	269	MET	C-N-CA	5.17	124.93	119.76

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	VAL	Peptide
1	A	126	SER	Peptide
1	A	213	LEU	Peptide
1	A	215	GLU	Peptide
1	A	218	ASN	Peptide
1	A	219	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	224	GLU	Peptide
1	A	300	GLU	Peptide
1	A	378	ASP	Peptide
1	A	390	GLU	Peptide
1	A	391	LEU	Peptide
1	A	408	ASN	Peptide
1	A	476	GLU	Peptide
1	A	477	ASN	Peptide
1	A	90	ALA	Peptide
1	B	101	ILE	Peptide
1	B	102	SER	Peptide
1	B	224	GLU	Peptide
1	B	282	ALA	Peptide
1	B	390	GLU	Peptide
1	B	431	LYS	Peptide
1	B	461	LYS	Peptide
1	B	475	GLU	Peptide
1	B	476	GLU	Peptide
1	B	481	VAL	Peptide
1	B	512	VAL	Peptide
1	B	96	SER	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	3097	0	3089	168	0
1	B	3013	0	3016	246	0
All	All	6110	0	6105	386	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 32.

All (386) 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:103:ALA:HB2	1:B:361:PHE:CE2	1.68	1.27
1:A:414:TYR:CD1	1:A:433:PHE:HZ	1.54	1.24
1:A:414:TYR:HD1	1:A:433:PHE:CZ	1.56	1.22
1:B:416:LYS:HD2	1:B:416:LYS:C	1.70	1.16
1:B:252:ASN:C	1:B:252:ASN:HD22	1.51	1.14
1:B:475:GLU:O	1:B:475:GLU:HG2	1.44	1.14
1:B:336:LEU:HB3	1:B:495:PHE:CE1	1.84	1.11
1:A:418:THR:HG22	1:A:420:GLU:H	1.10	1.10
1:B:432:ARG:HH11	1:B:432:ARG:CG	1.62	1.08
1:B:269:MET:HE3	1:B:303:PHE:HB3	1.29	1.07
1:A:269:MET:CE	1:A:303:PHE:HB3	1.85	1.06
1:A:296:THR:HG22	1:A:298:LYS:H	1.17	1.05
1:A:327:ASN:HD21	1:B:330:ASN:ND2	1.54	1.05
1:B:296:THR:HG22	1:B:298:LYS:H	1.19	1.05
1:A:205:PHE:HD1	1:A:205:PHE:O	1.39	1.03
1:B:416:LYS:HD2	1:B:416:LYS:O	1.57	1.03
1:B:296:THR:HG22	1:B:298:LYS:N	1.73	1.03
1:A:508:MET:HE2	1:B:345:GLN:HE21	1.21	1.02
1:A:294:THR:CG2	1:A:295:PHE:H	1.72	1.01
1:B:269:MET:CE	1:B:303:PHE:HB3	1.90	1.01
1:A:330:ASN:HD22	1:B:327:ASN:HD21	1.09	1.00
1:B:336:LEU:HB3	1:B:495:PHE:CZ	1.96	1.00
1:B:432:ARG:NH1	1:B:432:ARG:HG2	1.56	1.00
1:B:336:LEU:CB	1:B:495:PHE:CE1	2.45	0.98
1:B:250:ARG:HG2	1:B:250:ARG:HH11	1.27	0.96
1:B:454:THR:CG2	1:B:496:VAL:HG21	1.97	0.95
1:A:294:THR:CG2	1:A:295:PHE:N	2.27	0.94
1:B:393:LYS:O	1:B:394:SER:HB3	1.64	0.94
1:A:294:THR:HG23	1:A:295:PHE:H	1.32	0.94
1:A:327:ASN:ND2	1:B:330:ASN:ND2	2.16	0.93
1:A:414:TYR:HE2	1:A:418:THR:OG1	1.52	0.93
1:A:294:THR:HG22	1:A:295:PHE:N	1.84	0.92
1:B:102:SER:O	1:B:104:SER:N	2.02	0.92
1:B:370:PHE:CD1	1:B:412:ALA:HB2	2.04	0.92
1:A:512:VAL:HG21	1:B:509:TYR:CE1	2.05	0.91
1:B:432:ARG:HH11	1:B:432:ARG:HG2	0.78	0.91
1:B:252:ASN:C	1:B:252:ASN:ND2	2.27	0.91
1:B:148:GLN:NE2	1:B:148:GLN:HA	1.86	0.90
1:B:336:LEU:CB	1:B:495:PHE:HE1	1.83	0.90
1:B:458:ASN:HD22	1:B:458:ASN:H	1.15	0.89
1:A:418:THR:HG22	1:A:420:GLU:N	1.88	0.88
1:A:414:TYR:CD1	1:A:433:PHE:CZ	2.41	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ASN:ND2	1:B:327:ASN:HD21	1.71	0.87
1:B:449:ARG:H	1:B:472:ASN:HD21	1.20	0.87
1:B:475:GLU:O	1:B:475:GLU:CG	2.21	0.87
1:A:296:THR:HB	1:A:299:ASP:H	1.39	0.86
1:B:416:LYS:C	1:B:416:LYS:CD	2.48	0.86
1:A:205:PHE:O	1:A:205:PHE:CD1	2.27	0.86
1:B:168:LEU:O	1:B:172:ILE:HG13	1.76	0.86
1:B:269:MET:HE3	1:B:303:PHE:CB	2.07	0.85
1:B:296:THR:CG2	1:B:298:LYS:H	1.90	0.85
1:A:258:ILE:HG22	1:A:259:THR:CG2	2.07	0.84
1:B:103:ALA:CB	1:B:361:PHE:CE2	2.58	0.84
1:A:330:ASN:HD22	1:B:327:ASN:ND2	1.76	0.83
1:A:327:ASN:HD22	1:B:327:ASN:HD22	1.24	0.82
1:B:296:THR:HG22	1:B:297:GLU:N	1.94	0.82
1:B:296:THR:CG2	1:B:297:GLU:N	2.42	0.82
1:B:250:ARG:HH11	1:B:250:ARG:CG	1.93	0.82
1:B:376:CYS:O	1:B:377:SER:HB2	1.80	0.81
1:B:336:LEU:HB2	1:B:495:PHE:HE1	1.44	0.81
1:B:362:MET:HE3	1:B:362:MET:HA	1.61	0.81
1:B:370:PHE:HD2	1:B:383:VAL:HG22	1.43	0.81
1:B:91:MET:O	1:B:94:MET:N	2.13	0.80
1:A:378:ASP:OD1	1:A:378:ASP:C	2.26	0.79
1:A:269:MET:HE3	1:A:303:PHE:HB3	1.64	0.79
1:A:101:ILE:HD11	1:A:332:VAL:HG21	1.64	0.79
1:B:252:ASN:ND2	1:B:254:GLU:H	1.82	0.78
1:A:327:ASN:ND2	1:B:330:ASN:HD22	1.82	0.77
1:A:258:ILE:HG22	1:A:259:THR:HG23	1.64	0.77
1:B:419:MET:O	1:B:420:GLU:HG2	1.85	0.76
1:A:241:ASN:HD22	1:A:241:ASN:C	1.94	0.75
1:A:296:THR:HG22	1:A:298:LYS:N	1.98	0.75
1:B:101:ILE:HA	1:B:105:GLU:OE2	1.88	0.74
1:B:454:THR:HG21	1:B:496:VAL:HG21	1.69	0.74
1:A:458:ASN:H	1:A:458:ASN:HD22	1.36	0.74
1:B:370:PHE:CD2	1:B:383:VAL:HG22	2.23	0.73
1:B:103:ALA:HB2	1:B:361:PHE:HE2	1.42	0.73
1:B:376:CYS:O	1:B:377:SER:CB	2.36	0.73
1:B:101:ILE:HD12	1:B:101:ILE:O	1.89	0.72
1:A:508:MET:HE2	1:B:345:GLN:NE2	2.00	0.72
1:A:519:ARG:HB2	1:A:520:ASN:HD22	1.55	0.71
1:A:105:GLU:OE2	1:B:130:LYS:HB3	1.90	0.71
1:A:519:ARG:HB2	1:A:520:ASN:ND2	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:THR:HG22	1:B:496:VAL:HG21	1.73	0.71
1:A:448:ILE:O	1:A:448:ILE:HG22	1.90	0.70
1:B:269:MET:HE3	1:B:303:PHE:CD1	2.26	0.70
1:A:101:ILE:HD11	1:A:332:VAL:CG2	2.21	0.70
1:B:252:ASN:HD22	1:B:253:ALA:N	1.89	0.70
1:A:200:LEU:N	1:A:200:LEU:CD2	2.54	0.70
1:A:303:PHE:O	1:A:307:LEU:HG	1.92	0.70
1:A:520:ASN:HD22	1:A:520:ASN:N	1.90	0.69
1:B:112:PRO:HA	1:B:490:GLN:HE22	1.57	0.69
1:A:153:LEU:HD23	1:B:153:LEU:HD23	1.73	0.69
1:A:418:THR:CG2	1:A:420:GLU:H	1.98	0.69
1:A:508:MET:CE	1:B:345:GLN:HE21	2.03	0.69
1:B:393:LYS:O	1:B:394:SER:CB	2.41	0.69
1:B:294:THR:HG23	1:B:295:PHE:N	2.06	0.69
1:B:370:PHE:CE1	1:B:412:ALA:HB2	2.28	0.69
1:A:106:PHE:O	1:A:487:ASN:ND2	2.26	0.68
1:B:332:VAL:O	1:B:336:LEU:HG	1.93	0.68
1:B:358:ILE:HG23	1:B:362:MET:HG3	1.76	0.68
1:A:378:ASP:OD1	1:A:378:ASP:O	2.12	0.67
1:A:200:LEU:N	1:A:200:LEU:HD22	2.10	0.67
1:A:414:TYR:CE2	1:A:418:THR:OG1	2.34	0.67
1:A:283:GLN:NE2	1:A:285:ILE:HD11	2.10	0.67
1:B:336:LEU:HB2	1:B:495:PHE:CE1	2.23	0.67
1:B:458:ASN:HB3	1:B:465:ILE:HG13	1.78	0.66
1:A:258:ILE:HG22	1:A:259:THR:HG22	1.78	0.66
1:A:105:GLU:CD	1:B:130:LYS:HB3	2.21	0.66
1:B:422:LEU:O	1:B:452:LEU:HA	1.95	0.66
1:A:462:ASN:C	1:A:462:ASN:HD22	2.04	0.66
1:B:91:MET:O	1:B:93:HIS:N	2.28	0.65
1:B:291:ASN:HD22	1:B:291:ASN:H	1.44	0.65
1:A:512:VAL:CG2	1:B:509:TYR:CE1	2.78	0.65
1:B:373:ASP:HB2	1:B:379:SER:HB3	1.78	0.65
1:A:351:LEU:HD11	1:A:371:ILE:HD11	1.79	0.65
1:A:269:MET:HE1	1:A:303:PHE:HB3	1.77	0.64
1:B:448:ILE:CD1	1:B:448:ILE:H	2.09	0.64
1:B:103:ALA:HB2	1:B:361:PHE:CD2	2.29	0.64
1:A:159:ILE:HG22	1:A:171:LYS:HG2	1.79	0.64
1:A:153:LEU:CD2	1:B:153:LEU:HD23	2.26	0.64
1:A:269:MET:HE1	1:A:300:GLU:O	1.97	0.64
1:A:217:SER:O	1:A:218:ASN:HB2	1.97	0.64
1:A:195:SER:O	1:A:196:ASN:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:SER:C	1:B:104:SER:H	2.04	0.64
1:B:414:TYR:O	1:B:418:THR:OG1	2.16	0.64
1:B:250:ARG:CG	1:B:250:ARG:NH1	2.56	0.63
1:A:414:TYR:HD2	1:A:414:TYR:C	2.07	0.63
1:A:366:LYS:HG2	1:A:387:GLU:HG2	1.78	0.63
1:B:419:MET:C	1:B:420:GLU:HG2	2.24	0.63
1:A:489:GLU:O	1:A:493:GLU:HB2	1.98	0.63
1:A:296:THR:CG2	1:A:298:LYS:H	2.02	0.62
1:B:233:VAL:HG11	1:B:268:CYS:SG	2.40	0.62
1:B:385:HIS:CE1	1:B:387:GLU:OE2	2.53	0.62
1:B:147:ASP:HB3	1:B:150:SER:OG	2.00	0.62
1:B:370:PHE:HD1	1:B:412:ALA:HB2	1.61	0.61
1:B:385:HIS:HE1	1:B:387:GLU:OE2	1.82	0.61
1:A:327:ASN:HD21	1:B:330:ASN:HD21	1.44	0.61
1:A:426:ASP:OD1	1:A:426:ASP:C	2.43	0.61
1:B:362:MET:HA	1:B:362:MET:CE	2.32	0.60
1:B:428:SER:O	1:B:429:LYS:CG	2.50	0.60
1:B:518:LYS:C	1:B:520:ASN:H	2.09	0.60
1:B:269:MET:HE3	1:B:303:PHE:CG	2.35	0.60
1:A:446:GLN:C	1:A:447:CYS:SG	2.84	0.60
1:A:345:GLN:HE22	1:B:505:ASN:ND2	1.99	0.60
1:A:511:ALA:HA	1:A:514:ARG:NH1	2.18	0.59
1:A:388:CYS:C	1:A:390:GLU:H	2.10	0.59
1:A:462:ASN:ND2	1:A:463:LYS:HB2	2.18	0.59
1:B:294:THR:CG2	1:B:295:PHE:N	2.65	0.59
1:A:499:CYS:O	1:A:503:ILE:HG13	2.02	0.59
1:B:448:ILE:HG22	1:B:448:ILE:O	2.02	0.59
1:B:428:SER:O	1:B:429:LYS:CD	2.50	0.59
1:A:414:TYR:C	1:A:414:TYR:CD2	2.78	0.59
1:A:252:ASN:HD21	1:A:254:GLU:HG3	1.67	0.59
1:B:111:ARG:HE	1:B:326:GLU:CD	2.09	0.59
1:B:510:GLU:O	1:B:513:GLU:HB3	2.03	0.59
1:B:269:MET:HE1	1:B:300:GLU:O	2.02	0.58
1:B:427:VAL:HG12	1:B:428:SER:N	2.18	0.58
1:B:464:VAL:O	1:B:464:VAL:HG12	2.03	0.58
1:B:481:VAL:CG1	1:B:482:LYS:H	2.17	0.58
1:A:116:LYS:HB3	1:A:120:GLY:HA2	1.86	0.58
1:B:269:MET:CE	1:B:303:PHE:HD1	2.16	0.58
1:A:342:GLU:HG2	1:A:343:GLU:HG3	1.86	0.58
1:B:101:ILE:HD12	1:B:101:ILE:C	2.29	0.58
1:B:181:SER:O	1:B:287:LYS:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ALA:HB3	1:A:92:GLU:H	1.68	0.57
1:B:269:MET:CE	1:B:303:PHE:CD1	2.88	0.57
1:B:184:ARG:NH2	1:B:261:TYR:CD1	2.72	0.57
1:B:262:LYS:HE3	1:B:264:GLN:OE1	2.05	0.57
1:B:296:THR:CG2	1:B:297:GLU:H	2.18	0.57
1:A:454:THR:CG2	1:A:455:PRO:HD2	2.35	0.57
1:B:173:PHE:O	1:B:176:ILE:HG12	2.05	0.57
1:B:424:ILE:HD12	1:B:451:LEU:CD2	2.34	0.57
1:B:370:PHE:CD1	1:B:412:ALA:CB	2.84	0.57
1:B:428:SER:O	1:B:429:LYS:HD2	2.05	0.57
1:B:254:GLU:O	1:B:258:ILE:HG13	2.04	0.56
1:B:424:ILE:HD12	1:B:451:LEU:HD23	1.87	0.56
1:B:458:ASN:O	1:B:459:GLY:C	2.49	0.56
1:B:517:ALA:O	1:B:520:ASN:HB2	2.05	0.56
1:B:499:CYS:O	1:B:500:GLY:C	2.47	0.56
1:B:481:VAL:CG1	1:B:482:LYS:N	2.68	0.56
1:A:454:THR:HG23	1:A:455:PRO:HD2	1.87	0.56
1:B:371:ILE:HD12	1:B:371:ILE:N	2.21	0.55
1:B:108:ARG:HB2	1:B:109:PRO:HD2	1.88	0.55
1:A:272:LYS:O	1:A:311:GLY:HA3	2.07	0.55
1:A:331:GLN:HB3	1:B:125:LEU:HD23	1.88	0.55
1:B:448:ILE:CD1	1:B:448:ILE:N	2.69	0.55
1:A:105:GLU:OE2	1:B:130:LYS:HD3	2.07	0.55
1:A:269:MET:CE	1:A:303:PHE:HD1	2.19	0.55
1:A:418:THR:HG22	1:A:419:MET:N	2.20	0.55
1:A:267:LEU:O	1:A:283:GLN:HA	2.08	0.54
1:A:168:LEU:HD23	1:A:314:LEU:HD23	1.89	0.54
1:A:283:GLN:HE21	1:A:285:ILE:HD11	1.71	0.54
1:B:252:ASN:HD21	1:B:254:GLU:H	1.56	0.54
1:B:296:THR:HB	1:B:299:ASP:OD1	2.08	0.54
1:A:153:LEU:CD2	1:B:153:LEU:CD2	2.86	0.53
1:B:94:MET:O	1:B:94:MET:HG2	2.07	0.53
1:B:269:MET:HG3	1:B:303:PHE:CD1	2.44	0.53
1:A:299:ASP:C	1:A:301:LYS:H	2.16	0.53
1:B:230:VAL:HG23	1:B:231:GLY:N	2.23	0.53
1:B:388:CYS:SG	1:B:388:CYS:O	2.67	0.53
1:B:481:VAL:HG12	1:B:482:LYS:N	2.24	0.53
1:A:373:ASP:HA	1:A:381:SER:HB3	1.91	0.53
1:B:109:PRO:C	1:B:110:LEU:HD23	2.33	0.53
1:B:113:ILE:HD11	1:B:333:LEU:HD11	1.90	0.53
1:B:475:GLU:O	1:B:477:ASN:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ASN:ND2	1:B:484:PHE:HB2	2.24	0.52
1:A:223:LEU:HD13	1:A:230:VAL:HG22	1.90	0.52
1:B:384:PHE:CD2	1:B:385:HIS:N	2.77	0.52
1:B:447:CYS:O	1:B:449:ARG:N	2.43	0.52
1:B:458:ASN:HD22	1:B:458:ASN:N	1.89	0.52
1:B:109:PRO:O	1:B:110:LEU:HD23	2.10	0.52
1:B:410:MET:O	1:B:413:GLN:HB2	2.10	0.52
1:B:448:ILE:N	1:B:448:ILE:HD12	2.25	0.52
1:B:229:ILE:O	1:B:233:VAL:HG12	2.10	0.52
1:B:273:ASN:C	1:B:273:ASN:OD1	2.52	0.52
1:B:424:ILE:HD12	1:B:451:LEU:HB3	1.91	0.52
1:B:411:TYR:HB2	1:B:469:GLN:OE1	2.09	0.52
1:B:427:VAL:O	1:B:429:LYS:N	2.41	0.52
1:A:415:VAL:O	1:A:419:MET:N	2.36	0.52
1:B:339:LEU:O	1:B:340:ILE:C	2.52	0.52
1:B:368:THR:HG22	1:B:384:PHE:O	2.10	0.52
1:A:269:MET:CE	1:A:303:PHE:CD1	2.94	0.51
1:B:448:ILE:H	1:B:448:ILE:HD13	1.76	0.51
1:A:344:GLN:H	1:B:505:ASN:HD21	1.58	0.51
1:B:296:THR:HG23	1:B:297:GLU:H	1.75	0.51
1:A:269:MET:HE3	1:A:303:PHE:CD1	2.46	0.51
1:B:99:ARG:HE	1:B:99:ARG:HA	1.76	0.51
1:A:516:MET:HG3	1:B:516:MET:HG3	1.92	0.51
1:B:454:THR:HG21	1:B:496:VAL:CG2	2.38	0.51
1:B:512:VAL:O	1:B:513:GLU:C	2.54	0.50
1:B:350:ILE:CG2	1:B:351:LEU:N	2.74	0.50
1:A:223:LEU:CD1	1:A:230:VAL:HG22	2.42	0.50
1:B:450:SER:H	1:B:472:ASN:ND2	2.09	0.50
1:A:452:LEU:HD13	1:A:492:LEU:HD23	1.92	0.50
1:A:153:LEU:HD23	1:B:153:LEU:CD2	2.40	0.50
1:A:241:ASN:C	1:A:241:ASN:ND2	2.65	0.50
1:A:269:MET:HE2	1:A:303:PHE:HD1	1.77	0.49
1:A:458:ASN:ND2	1:A:460:LYS:O	2.44	0.49
1:B:432:ARG:CG	1:B:432:ARG:NH1	2.35	0.49
1:B:432:ARG:C	1:B:433:PHE:CD2	2.90	0.49
1:B:458:ASN:H	1:B:458:ASN:ND2	1.97	0.49
1:A:179:LEU:HD13	1:A:303:PHE:HA	1.94	0.49
1:B:416:LYS:O	1:B:416:LYS:CD	2.44	0.49
1:A:388:CYS:C	1:A:390:GLU:N	2.71	0.49
1:A:346:SER:O	1:A:347:LEU:C	2.56	0.49
1:B:366:LYS:NZ	1:B:448:ILE:HD11	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HG22	1:A:101:ILE:O	2.12	0.49
1:A:324:LEU:HD22	1:B:129:GLU:HG2	1.95	0.48
1:A:462:ASN:HD22	1:A:463:LYS:HB2	1.78	0.48
1:B:110:LEU:HD12	1:B:329:ARG:NH1	2.27	0.48
1:A:452:LEU:HD22	1:A:453:CYS:H	1.77	0.48
1:B:238:GLU:OE2	1:B:239:PRO:HD2	2.13	0.48
1:A:414:TYR:HD2	1:A:414:TYR:O	1.97	0.48
1:B:428:SER:O	1:B:429:LYS:HG3	2.12	0.48
1:B:230:VAL:O	1:B:231:GLY:C	2.57	0.47
1:B:251:PHE:CG	1:B:252:ASN:N	2.82	0.47
1:B:252:ASN:HD22	1:B:254:GLU:H	1.61	0.47
1:A:368:THR:HG22	1:A:370:PHE:CE1	2.50	0.47
1:B:368:THR:HG23	1:B:385:HIS:CD2	2.49	0.47
1:B:108:ARG:HB2	1:B:109:PRO:CD	2.45	0.47
1:B:252:ASN:HD21	1:B:254:GLU:HB2	1.79	0.47
1:A:362:MET:HE2	1:A:362:MET:HB3	1.82	0.47
1:B:366:LYS:HZ3	1:B:448:ILE:HD11	1.79	0.47
1:B:458:ASN:HB3	1:B:465:ILE:CG1	2.42	0.47
1:A:273:ASN:OD1	1:A:273:ASN:C	2.57	0.47
1:A:173:PHE:O	1:A:176:ILE:HG12	2.14	0.47
1:B:269:MET:HE1	1:B:300:GLU:HA	1.97	0.47
1:B:269:MET:CE	1:B:303:PHE:CB	2.76	0.46
1:B:415:VAL:O	1:B:419:MET:N	2.39	0.46
1:A:433:PHE:HA	1:A:434:PRO:HD2	1.80	0.46
1:B:248:ASP:HA	1:B:249:PRO:HD2	1.67	0.46
1:B:433:PHE:HA	1:B:434:PRO:HD3	1.78	0.46
1:B:98:THR:O	1:B:98:THR:CG2	2.64	0.46
1:B:447:CYS:O	1:B:448:ILE:C	2.59	0.46
1:A:452:LEU:HD13	1:A:492:LEU:CD2	2.46	0.46
1:B:419:MET:HG2	1:B:464:VAL:HG21	1.98	0.46
1:A:462:ASN:C	1:A:462:ASN:ND2	2.70	0.45
1:B:467:VAL:CG1	1:B:468:CYS:N	2.79	0.45
1:B:264:GLN:H	1:B:264:GLN:HG2	1.59	0.45
1:B:275:ARG:NH1	1:B:277:GLU:OE2	2.50	0.45
1:B:433:PHE:CD2	1:B:433:PHE:N	2.84	0.45
1:A:430:ASP:OD1	1:A:430:ASP:C	2.60	0.45
1:B:370:PHE:HD2	1:B:383:VAL:CG2	2.23	0.45
1:A:184:ARG:HB3	1:A:206:ASP:HB2	1.99	0.45
1:A:184:ARG:HH22	1:A:208:ALA:HB2	1.82	0.45
1:A:327:ASN:HA	1:B:327:ASN:ND2	2.31	0.45
1:A:388:CYS:O	1:A:390:GLU:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ASP:HA	1:B:381:SER:HB3	1.98	0.45
1:B:464:VAL:O	1:B:465:ILE:C	2.60	0.45
1:B:230:VAL:CG2	1:B:231:GLY:N	2.80	0.45
1:A:347:LEU:O	1:A:351:LEU:HG	2.16	0.45
1:A:223:LEU:CD1	1:A:230:VAL:CG2	2.95	0.45
1:A:226:ASN:CG	1:A:226:ASN:O	2.59	0.45
1:A:366:LYS:HE2	1:A:387:GLU:OE2	2.16	0.45
1:A:520:ASN:ND2	1:A:520:ASN:N	2.60	0.45
1:B:205:PHE:N	1:B:205:PHE:CD2	2.84	0.45
1:B:91:MET:HG2	1:B:94:MET:HB3	2.00	0.44
1:B:458:ASN:HA	1:B:465:ILE:CD1	2.48	0.44
1:A:101:ILE:CD1	1:A:332:VAL:HG21	2.43	0.44
1:A:514:ARG:C	1:A:516:MET:H	2.26	0.44
1:B:380:PHE:HZ	1:B:412:ALA:HB1	1.82	0.44
1:B:518:LYS:C	1:B:520:ASN:N	2.72	0.44
1:A:246:TYR:CE2	1:A:262:LYS:HE2	2.53	0.44
1:A:351:LEU:CD1	1:A:371:ILE:HD11	2.47	0.44
1:A:452:LEU:HB2	1:A:484:PHE:CG	2.53	0.44
1:B:97:MET:SD	1:B:336:LEU:HD21	2.58	0.44
1:A:213:LEU:HB3	1:A:217:SER:CB	2.47	0.44
1:A:269:MET:CE	1:A:303:PHE:CB	2.76	0.44
1:B:100:LYS:C	1:B:101:ILE:HG23	2.43	0.44
1:B:380:PHE:CZ	1:B:412:ALA:HB1	2.53	0.44
1:A:127:ASP:HB2	1:B:100:LYS:NZ	2.32	0.44
1:B:486:ARG:HG3	1:B:486:ARG:HH11	1.82	0.44
1:B:303:PHE:O	1:B:307:LEU:HG	2.18	0.44
1:A:258:ILE:HG23	1:A:258:ILE:O	2.17	0.44
1:B:246:TYR:CD2	1:B:262:LYS:NZ	2.86	0.44
1:B:384:PHE:HD2	1:B:385:HIS:N	2.15	0.44
1:B:419:MET:O	1:B:420:GLU:CG	2.59	0.44
1:A:299:ASP:C	1:A:301:LYS:N	2.75	0.43
1:B:291:ASN:HD22	1:B:291:ASN:N	2.14	0.43
1:B:432:ARG:C	1:B:433:PHE:HD2	2.25	0.43
1:B:423:ASN:HD21	1:B:484:PHE:HB2	1.81	0.43
1:B:450:SER:H	1:B:472:ASN:HD22	1.65	0.43
1:B:460:LYS:O	1:B:461:LYS:HB2	2.18	0.43
1:A:512:VAL:CG2	1:B:509:TYR:HE1	2.29	0.43
1:B:253:ALA:O	1:B:254:GLU:C	2.62	0.43
1:B:269:MET:HE2	1:B:303:PHE:HD1	1.81	0.43
1:B:427:VAL:HG21	1:B:448:ILE:HG22	2.00	0.43
1:A:351:LEU:HD21	1:A:503:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:THR:HG23	1:B:295:PHE:H	1.82	0.43
1:A:118:SER:O	1:A:119:GLU:CB	2.67	0.43
1:A:496:VAL:HA	1:A:499:CYS:HB2	2.01	0.43
1:B:172:ILE:HD13	1:B:310:CYS:SG	2.59	0.43
1:B:368:THR:CG2	1:B:384:PHE:O	2.66	0.43
1:B:275:ARG:O	1:B:276:GLU:HB2	2.19	0.43
1:A:365:GLN:HG2	1:A:474:MET:HE2	2.00	0.42
1:B:116:LYS:CG	1:B:122:VAL:HG12	2.48	0.42
1:A:195:SER:O	1:A:196:ASN:CB	2.67	0.42
1:A:205:PHE:CD1	1:A:205:PHE:C	2.87	0.42
1:A:381:SER:OG	1:A:382:SER:N	2.53	0.42
1:B:99:ARG:HA	1:B:99:ARG:NE	2.34	0.42
1:B:481:VAL:HG13	1:B:482:LYS:H	1.84	0.42
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.71	0.42
1:A:200:LEU:CD2	1:A:200:LEU:H	2.29	0.42
1:B:195:SER:C	1:B:196:ASN:HD22	2.27	0.42
1:B:372:VAL:CG1	1:B:373:ASP:N	2.80	0.42
1:B:112:PRO:HA	1:B:490:GLN:NE2	2.28	0.42
1:A:336:LEU:O	1:A:340:ILE:HG23	2.20	0.42
1:B:98:THR:O	1:B:98:THR:HG22	2.19	0.42
1:B:148:GLN:NE2	1:B:148:GLN:CA	2.68	0.42
1:A:336:LEU:HD13	1:A:357:THR:HG21	2.01	0.42
1:B:91:MET:O	1:B:92:GLU:C	2.63	0.42
1:A:171:LYS:HE2	1:A:171:LYS:HB2	1.75	0.42
1:A:214:GLU:O	1:A:217:SER:HB3	2.19	0.42
1:A:151:ARG:HA	1:A:151:ARG:HD2	1.76	0.42
1:A:184:ARG:HB3	1:A:206:ASP:CB	2.49	0.42
1:B:368:THR:HG23	1:B:385:HIS:HD2	1.85	0.42
1:A:200:LEU:H	1:A:200:LEU:HD23	1.84	0.42
1:A:252:ASN:ND2	1:A:254:GLU:HG3	2.35	0.42
1:A:351:LEU:O	1:A:352:LYS:C	2.62	0.42
1:B:269:MET:HE1	1:B:303:PHE:HB3	1.91	0.42
1:A:184:ARG:NH2	1:A:208:ALA:HB2	2.35	0.41
1:A:269:MET:HE2	1:A:303:PHE:CD1	2.55	0.41
1:A:352:LYS:NZ	1:A:352:LYS:HB3	2.35	0.41
1:A:460:LYS:H	1:A:460:LYS:HG2	1.47	0.41
1:B:473:LYS:HB3	1:B:482:LYS:O	2.21	0.41
1:A:213:LEU:HB3	1:A:217:SER:HB3	2.03	0.41
1:B:462:ASN:HB3	1:B:463:LYS:H	1.62	0.41
1:A:213:LEU:CD2	1:A:217:SER:HB2	2.50	0.41
1:A:458:ASN:H	1:A:458:ASN:ND2	2.11	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ALA:CB	1:B:361:PHE:HE2	2.17	0.41
1:B:478:THR:HG21	1:B:480:LYS:HB2	2.02	0.41
1:A:285:ILE:O	1:A:286:ASN:HB2	2.21	0.41
1:A:347:LEU:O	1:A:350:ILE:HG22	2.21	0.41
1:A:407:ILE:O	1:A:409:TYR:CD2	2.74	0.41
1:A:428:SER:C	1:A:430:ASP:H	2.29	0.41
1:B:180:ILE:HD13	1:B:180:ILE:N	2.35	0.41
1:B:267:LEU:HD21	1:B:269:MET:HE2	2.02	0.41
1:B:358:ILE:HG21	1:B:470:LEU:HD21	2.02	0.41
1:B:92:GLU:C	1:B:94:MET:N	2.76	0.40
1:B:148:GLN:HA	1:B:148:GLN:HE21	1.80	0.40
1:B:350:ILE:HG23	1:B:351:LEU:N	2.35	0.40
1:B:412:ALA:O	1:B:413:GLN:C	2.63	0.40
1:A:423:ASN:OD1	1:A:423:ASN:C	2.64	0.40
1:B:239:PRO:O	1:B:240:LEU:HD23	2.21	0.40
1:B:450:SER:OG	1:B:472:ASN:HA	2.22	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	383/431 (89%)	335 (88%)	41 (11%)	7 (2%)	6	23
1	B	370/431 (86%)	303 (82%)	51 (14%)	16 (4%)	2	7
All	All	753/862 (87%)	638 (85%)	92 (12%)	23 (3%)	3	12

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	VAL
1	A	390	GLU

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Mol	Chain	Res	Type
1	A	477	ASN
1	B	103	ALA
1	B	339	LEU
1	B	340	ILE
1	B	377	SER
1	B	429	LYS
1	B	448	ILE
1	B	465	ILE
1	B	513	GLU
1	A	378	ASP
1	A	389	GLU
1	B	95	ALA
1	B	127	ASP
1	B	500	GLY
1	A	115	VAL
1	B	93	HIS
1	B	428	SER
1	B	462	ASN
1	B	519	ARG
1	A	448	ILE
1	B	425	PRO

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	349/387 (90%)	287 (82%)	62 (18%)	2	6
1	B	340/387 (88%)	269 (79%)	71 (21%)	1	4
All	All	689/774 (89%)	556 (81%)	133 (19%)	1	5

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LYS
1	A	101	ILE

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Mol	Chain	Res	Type
1	A	115	VAL
1	A	119	GLU
1	A	122	VAL
1	A	125	LEU
1	A	149	SER
1	A	150	SER
1	A	181	SER
1	A	194	SER
1	A	200	LEU
1	A	205	PHE
1	A	209	GLU
1	A	211	SER
1	A	213	LEU
1	A	219	ASN
1	A	223	LEU
1	A	227	LYS
1	A	230	VAL
1	A	242	ILE
1	A	243	LYS
1	A	258	ILE
1	A	264	GLN
1	A	269	MET
1	A	289	SER
1	A	294	THR
1	A	303	PHE
1	A	326	GLU
1	A	328	LYS
1	A	333	LEU
1	A	339	LEU
1	A	342	GLU
1	A	352	LYS
1	A	354	ILE
1	A	374	GLU
1	A	378	ASP
1	A	381	SER
1	A	391	LEU
1	A	392	GLU
1	A	408	ASN
1	A	410	MET
1	A	414	TYR
1	A	418	THR
1	A	422	LEU

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Mol	Chain	Res	Type
1	A	427	VAL
1	A	430	ASP
1	A	447	CYS
1	A	448	ILE
1	A	449	ARG
1	A	451	LEU
1	A	452	LEU
1	A	458	ASN
1	A	460	LYS
1	A	461	LYS
1	A	462	ASN
1	A	473	LYS
1	A	477	ASN
1	A	480	LYS
1	A	503	ILE
1	A	512	VAL
1	A	519	ARG
1	A	520	ASN
1	B	96	SER
1	B	99	ARG
1	B	100	LYS
1	B	105	GLU
1	B	108	ARG
1	B	119	GLU
1	B	121	THR
1	B	123	SER
1	B	129	GLU
1	B	148	GLN
1	B	157	LYS
1	B	172	ILE
1	B	180	ILE
1	B	200	LEU
1	B	201	ILE
1	B	207	VAL
1	B	233	VAL
1	B	236	LEU
1	B	242	ILE
1	B	248	ASP
1	B	250	ARG
1	B	252	ASN
1	B	254	GLU
1	B	258	ILE

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Mol	Chain	Res	Type
1	B	264	GLN
1	B	269	MET
1	B	277	GLU
1	B	283	GLN
1	B	291	ASN
1	B	294	THR
1	B	297	GLU
1	B	301	LYS
1	B	338	SER
1	B	339	LEU
1	B	342	GLU
1	B	345	GLN
1	B	346	SER
1	B	352	LYS
1	B	357	THR
1	B	359	ILE
1	B	360	SER
1	B	362	MET
1	B	368	THR
1	B	383	VAL
1	B	387	GLU
1	B	389	GLU
1	B	390	GLU
1	B	391	LEU
1	B	410	MET
1	B	416	LYS
1	B	418	THR
1	B	424	ILE
1	B	427	VAL
1	B	429	LYS
1	B	430	ASP
1	B	431	LYS
1	B	432	ARG
1	B	447	CYS
1	B	448	ILE
1	B	453	CYS
1	B	454	THR
1	B	458	ASN
1	B	463	LYS
1	B	475	GLU
1	B	480	LYS
1	B	496	VAL

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Mol	Chain	Res	Type
1	B	504	GLN
1	B	508	MET
1	B	514	ARG
1	B	516	MET
1	B	518	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	170	HIS
1	A	218	ASN
1	A	219	ASN
1	A	241	ASN
1	A	252	ASN
1	A	264	GLN
1	A	274	HIS
1	A	283	GLN
1	A	315	HIS
1	A	344	GLN
1	A	413	GLN
1	A	458	ASN
1	A	462	ASN
1	A	469	GLN
1	A	487	ASN
1	A	505	ASN
1	A	520	ASN
1	B	148	GLN
1	B	196	ASN
1	B	219	ASN
1	B	252	ASN
1	B	257	GLN
1	B	283	GLN
1	B	291	ASN
1	B	315	HIS
1	B	318	GLN
1	B	327	ASN
1	B	330	ASN
1	B	344	GLN
1	B	345	GLN
1	B	385	HIS
1	B	458	ASN

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Mol	Chain	Res	Type
1	B	472	ASN
1	B	490	GLN
1	B	505	ASN
1	B	520	ASN

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	391/431 (90%)	0.27	18 (4%) 37 29	43, 77, 123, 156	0
1	B	380/431 (88%)	0.50	29 (7%) 20 14	48, 83, 132, 181	0
All	All	771/862 (89%)	0.39	47 (6%) 27 20	43, 79, 129, 181	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	GLU	6.5
1	B	434	PRO	6.2
1	A	391	LEU	6.1
1	B	90	ALA	6.0
1	A	216	VAL	6.0
1	B	93	HIS	5.5
1	B	409	TYR	5.1
1	B	391	LEU	4.9
1	B	130	LYS	4.9
1	B	97	MET	4.8
1	B	128	SER	4.6
1	A	407	ILE	4.4
1	A	212	THR	4.2
1	B	433	PHE	3.8
1	A	90	ALA	3.7
1	A	394	SER	3.6
1	A	435	TRP	3.5
1	A	213	LEU	3.3
1	B	208	ALA	3.2
1	A	205	PHE	3.2
1	B	393	LYS	2.8
1	A	393	LYS	2.8
1	A	520	ASN	2.6
1	B	377	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	411	TYR	2.6
1	B	91	MET	2.5
1	B	345	GLN	2.5
1	B	366	LYS	2.5
1	A	219	ASN	2.5
1	B	394	SER	2.4
1	A	247	GLU	2.3
1	B	103	ALA	2.3
1	B	460	LYS	2.3
1	A	449	ARG	2.3
1	A	249	PRO	2.3
1	B	95	ALA	2.3
1	B	223	LEU	2.2
1	A	146	GLY	2.2
1	B	495	PHE	2.2
1	A	274	HIS	2.2
1	A	91	MET	2.2
1	B	511	ALA	2.2
1	B	379	SER	2.1
1	B	491	PHE	2.1
1	B	469	GLN	2.1
1	B	205	PHE	2.1
1	B	448	ILE	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.