



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:15 AM GMT

PDB ID : 3LFV
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

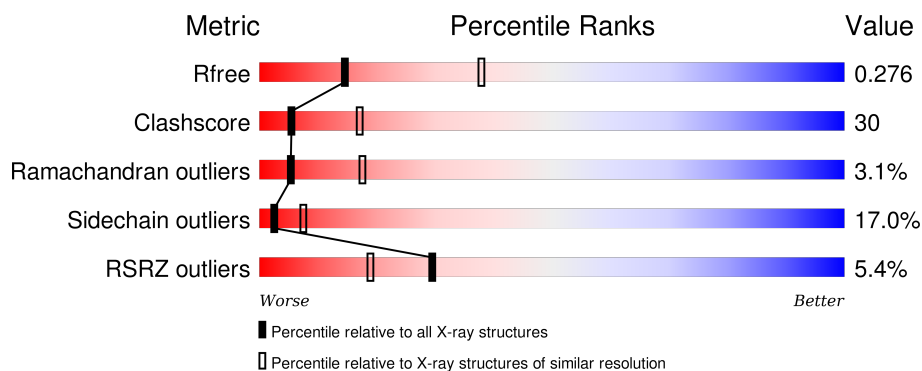
1 Overall quality at a glance ⓘ

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>6%</div> <div> <div></div> <div>55%</div> <div>29%</div> <div>7%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	431	<div> <div>4%</div> <div> <div></div> <div>41%</div> <div>34%</div> <div>12%</div> <div>•</div> <div>12%</div> </div> </div>

2 Entry composition [i](#)

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			

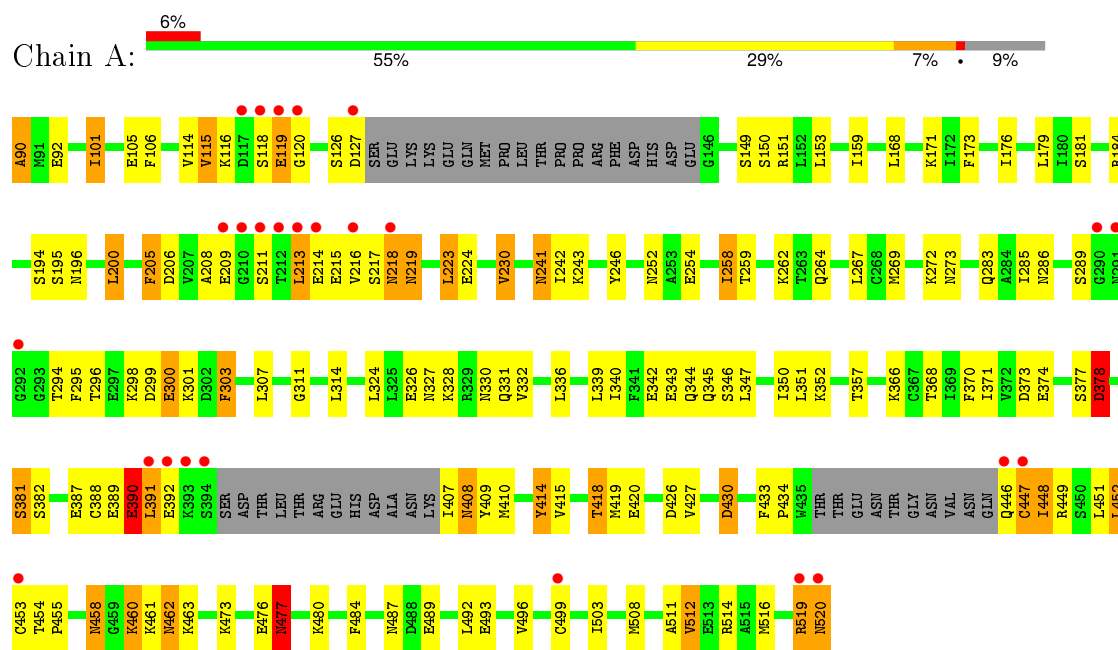
There are 22 discrepancies between the modelled and reference sequences:

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	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	UNP O76074
B	519	ARG	-	expression tag	UNP O76074
B	520	ASN	-	expression tag	UNP O76074

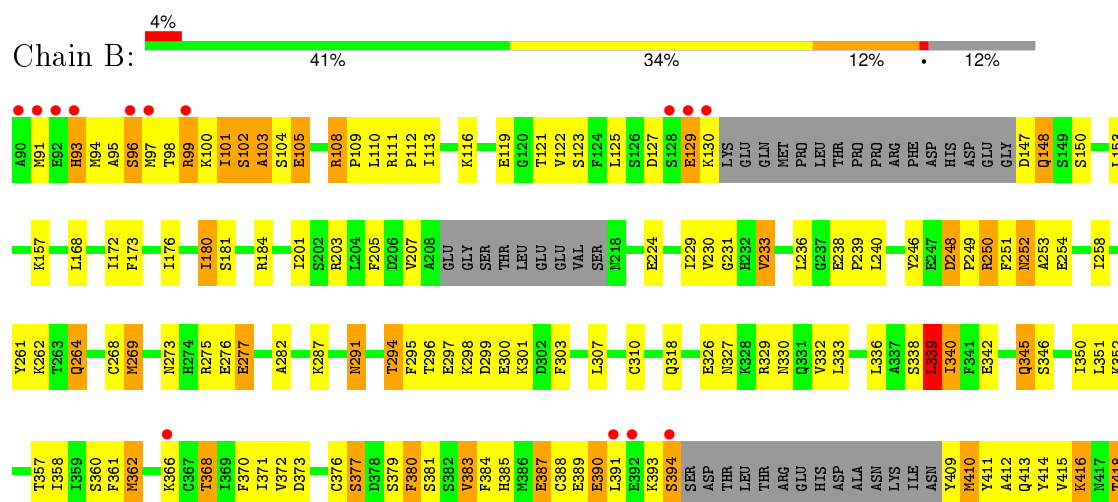
3 Residue-property plots

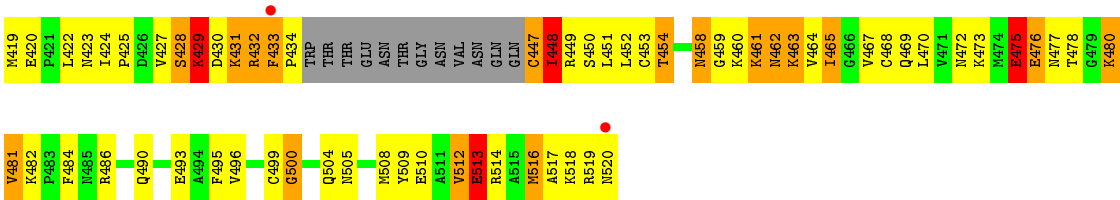
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: cGMP-specific 3',5'-cyclic phosphodiesterase



- Molecule 1: cGMP-specific 3',5'-cyclic phosphodiesterase





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 29.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.80) 99.2 (29.67-2.70)	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 5.5.0109	Depositor
R, R_{free}	0.240 , 0.285 0.234 , 0.276	Depositor DCC
R_{free} test set	2034 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.0	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44457 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.32	0/3145	0.42	0/4232
1	B	0.31	0/3058	0.41	0/4110
All	All	0.31	0/6203	0.42	0/8342

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.

There are no bond angle outliers.

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
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

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Mol	Chain	Res	Type	Group
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	158	0
1	B	3013	0	3016	234	0
All	All	6110	0	6105	364	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 30.

All (364) 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:475:GLU:O	1:B:475:GLU:HG2	1.44	1.14
1:B:269:MET:HE3	1:B:303:PHE:HB3	1.19	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:HB3	1:B:495:PHE:CE1	1.84	1.11
1:B:416:LYS:C	1:B:416:LYS:HD2	1.70	1.11
1:A:418:THR:HG22	1:A:420:GLU:H	1.10	1.10
1:B:252:ASN:HD22	1:B:252:ASN:C	1.51	1.09
1:B:432:ARG:CG	1:B:432:ARG:HH11	1.62	1.08
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:B:416:LYS:O	1:B:416:LYS:HD2	1.57	1.03
1:A:205:PHE:HD1	1:A:205:PHE:O	1.39	1.03
1:B:296:THR:HG22	1:B:298:LYS:N	1.73	1.03
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:HG2	1:B:432:ARG:HH11	0.78	0.91
1:B:148:GLN:HA	1:B:148:GLN:NE2	1.86	0.90
1:B:336:LEU:CB	1:B:495:PHE:HE1	1.83	0.90
1:B:458:ASN:H	1:B:458:ASN:HD22	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
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:A:205:PHE:CD1	1:A:205:PHE:O	2.27	0.86
1:B:252:ASN:ND2	1:B:252:ASN:C	2.27	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LEU:O	1:B:172:ILE:HG13	1.76	0.86
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:B:269:MET:HE3	1:B:303:PHE:CB	2.07	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: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:B:362:MET:HE3	1:B:362:MET:HA	1.63	0.80
1:A:269:MET:HE3	1:A:303:PHE:HB3	1.65	0.79
1:B:269:MET:HE2	1:B:303:PHE:HD1	1.47	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:B:416:LYS:C	1:B:416:LYS:CD	2.48	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:296:THR:HG22	1:A:298:LYS:N	1.98	0.75
1:A:378:ASP:OD1	1:A:378:ASP:C	2.26	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:CE	1:B:345:GLN:HE21	2.03	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
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:252:ASN:HD22	1:B:253:ALA:N	1.89	0.70
1:A:101:ILE:HD11	1:A:332:VAL:CG2	2.21	0.70
1:A:241:ASN:HD22	1:A:241:ASN:C	1.94	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:269:MET:HE1	1:B:300:GLU:HA	1.72	0.69
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:418:THR:CG2	1:A:420:GLU:H	1.98	0.69
1:B:393:LYS:O	1:B:394:SER:CB	2.41	0.69
1:A:153:LEU:HD23	1:B:153:LEU:HD23	1.73	0.69
1:B:370:PHE:CE1	1:B:412:ALA:HB2	2.28	0.69
1:B:294:THR:HG23	1:B:295:PHE:N	2.06	0.69
1:A:508:MET:HE2	1:B:345:GLN:HE21	1.58	0.69
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:106:PHE:O	1:A:487:ASN:ND2	2.26	0.68
1:A:378:ASP:O	1:A:378:ASP:OD1	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:B:336:LEU:HB2	1:B:495:PHE:CE1	2.23	0.67
1:A:283:GLN:NE2	1:A:285:ILE:HD11	2.10	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:B:422:LEU:O	1:B:452:LEU:HA	1.95	0.66
1:B:91:MET:O	1:B:93:HIS:N	2.28	0.65
1:B:291:ASN:H	1:B:291:ASN:HD22	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:H	1:B:448:ILE:CD1	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: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
1:A:269:MET:HE1	1:A:300:GLU:O	1.98	0.64
1:B:414:TYR:O	1:B:418:THR:OG1	2.16	0.64
1:B:250:ARG:NH1	1:B:250:ARG:CG	2.56	0.63
1:A:366:LYS:HG2	1:A:387:GLU:HG2	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:269:MET:HE2	1:B:303:PHE:CD1	2.33	0.62
1:B:370:PHE:HD1	1:B:412:ALA:HB2	1.61	0.61
1:A:105:GLU:CD	1:B:130:LYS:HB3	2.21	0.61
1:B:385:HIS:HE1	1:B:387:GLU:OE2	1.82	0.61
1:A:462:ASN:C	1:A:462:ASN:HD22	2.04	0.61
1:A:327:ASN:HD21	1:B:330:ASN:HD21	1.44	0.61
1:B:428:SER:O	1:B:429:LYS:CG	2.50	0.60
1:B:362:MET:CE	1:B:362:MET:HA	2.32	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:B:294:THR:CG2	1:B:295:PHE:N	2.65	0.59
1:A:462:ASN:ND2	1:A:463:LYS:HB2	2.18	0.59
1:B:448:ILE:HG22	1:B:448:ILE:O	2.02	0.59
1:A:499:CYS:O	1:A:503:ILE:HG13	2.02	0.59
1:B:428:SER:O	1:B:429:LYS:CD	2.50	0.59
1:A:252:ASN:HD21	1:A:254:GLU:HG3	1.67	0.59
1:B:510:GLU:O	1:B:513:GLU:HB3	2.03	0.59
1:A:414:TYR:C	1:A:414:TYR:HD2	2.07	0.58
1:B:464:VAL:HG12	1:B:464:VAL:O	2.03	0.58
1:B:427:VAL:HG12	1:B:428:SER:N	2.18	0.58
1:B:419:MET:C	1:B:420:GLU:HG2	2.24	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:A:342:GLU:HG2	1:A:343:GLU:HG3	1.86	0.58
1:B:181:SER:O	1:B:287:LYS:HD2	2.04	0.57
1:B:269:MET:CE	1:B:303:PHE:CD1	2.88	0.57
1:A:90:ALA:HB3	1:A:92:GLU:H	1.68	0.57
1:B:262:LYS:HE3	1:B:264:GLN:OE1	2.05	0.57
1:B:184:ARG:NH2	1:B:261:TYR:CD1	2.72	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:424:ILE:HD12	1:B:451:LEU:CD2	2.34	0.57
1:B:173:PHE:O	1:B:176:ILE:HG12	2.05	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:517:ALA:O	1:B:520:ASN:HB2	2.05	0.56
1:A:426:ASP:OD1	1:A:426:ASP:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:518:LYS:C	1:B:520:ASN:H	2.09	0.55
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:331:GLN:HB3	1:B:125:LEU:HD23	1.88	0.55
1:A:272:LYS:O	1:A:311:GLY:HA3	2.07	0.55
1:B:448:ILE:N	1:B:448:ILE:CD1	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:B:269:MET:CE	1:B:303:PHE:HD1	2.16	0.54
1:A:388:CYS:C	1:A:390:GLU:H	2.10	0.54
1:A:414:TYR:C	1:A:414:TYR:CD2	2.78	0.54
1:A:446:GLN:C	1:A:447:CYS:SG	2.84	0.54
1:A:267:LEU:O	1:A:283:GLN:HA	2.08	0.54
1:B:111:ARG:HE	1:B:326:GLU:CD	2.09	0.54
1:A:168:LEU:HD23	1:A:314:LEU:HD23	1.89	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:283:GLN:HE21	1:A:285:ILE:HD11	1.71	0.54
1:B:94:MET:HG2	1:B:94:MET:O	2.07	0.53
1:A:153:LEU:CD2	1:B:153:LEU:CD2	2.86	0.53
1:B:269:MET:HG3	1:B:303:PHE:CD1	2.44	0.53
1:B:101:ILE:HD12	1:B:101:ILE:C	2.29	0.53
1:B:481:VAL:HG12	1:B:482:LYS:N	2.24	0.53
1:B:388:CYS:O	1:B:388:CYS:SG	2.67	0.53
1:B:230:VAL:HG23	1:B:231:GLY:N	2.23	0.53
1:A:373:ASP:HA	1:A:381:SER:HB3	1.91	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
1:B:423:ASN:ND2	1:B:484:PHE:HB2	2.24	0.52
1:A:269:MET:HE3	1:A:303:PHE:CD1	2.45	0.52
1:B:458:ASN:HD22	1:B:458:ASN:N	1.89	0.52
1:B:447:CYS:O	1:B:449:ARG:N	2.43	0.52
1:B:384:PHE:CD2	1:B:385:HIS:N	2.77	0.52
1:A:223:LEU:HD13	1:A:230:VAL:HG22	1.90	0.52
1:B:448:ILE:N	1:B:448:ILE:HD12	2.25	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:229:ILE:O	1:B:233:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ILE:HD12	1:B:451:LEU:HB3	1.91	0.52
1:B:458:ASN:O	1:B:459:GLY:C	2.49	0.52
1:B:427:VAL:O	1:B:429:LYS:N	2.41	0.52
1:B:411:TYR:HB2	1:B:469:GLN:OE1	2.09	0.52
1:A:415:VAL:O	1:A:419:MET:N	2.36	0.52
1:B:368:THR:HG22	1:B:384:PHE:O	2.10	0.52
1:B:499:CYS:O	1:B:500:GLY:C	2.47	0.51
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:B:296:THR:HG23	1:B:297:GLU:H	1.75	0.51
1:A:344:GLN:H	1:B:505:ASN:HD21	1.58	0.51
1:B:99:ARG:HA	1:B:99:ARG:HE	1.76	0.51
1:B:454:THR:HG21	1:B:496:VAL:CG2	2.38	0.51
1:A:516:MET:HG3	1:B:516:MET:HG3	1.92	0.51
1:B:350:ILE:CG2	1:B:351:LEU:N	2.74	0.50
1:B:450:SER:H	1:B:472:ASN:ND2	2.09	0.50
1:A:508:MET:HE1	1:B:345:GLN:HE21	1.76	0.50
1:A:223:LEU:CD1	1:A:230:VAL:HG22	2.42	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:B:432:ARG:CG	1:B:432:ARG:NH1	2.35	0.49
1:B:458:ASN:ND2	1:B:458:ASN:H	1.97	0.49
1:A:458:ASN:ND2	1:A:460:LYS:O	2.44	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:B:366:LYS:NZ	1:B:448:ILE:HD11	2.28	0.49
1:A:101:ILE:HG22	1:A:101:ILE:O	2.12	0.49
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:324:LEU:HD22	1:B:129:GLU:HG2	1.95	0.48
1:A:452:LEU:HD22	1:A:453:CYS:H	1.77	0.48
1:A:299:ASP:C	1:A:301:LYS:H	2.16	0.48
1:B:238:GLU:OE2	1:B:239:PRO:HD2	2.13	0.48
1:B:109:PRO:C	1:B:110:LEU:HD23	2.33	0.48
1:A:269:MET:HE2	1:A:303:PHE:HD1	1.79	0.48
1:A:414:TYR:O	1:A:414:TYR:HD2	1.97	0.48
1:B:428:SER:O	1:B:429:LYS:HG3	2.12	0.48
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:B:368:THR:HG23	1:B:385:HIS:CD2	2.49	0.47
1:B:273:ASN:OD1	1:B:273:ASN:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:THR:HG22	1:A:370:PHE:CE1	2.50	0.47
1:B:252:ASN:HD21	1:B:254:GLU:HB2	1.79	0.47
1:B:108:ARG:HB2	1:B:109:PRO:CD	2.45	0.47
1:B:458:ASN:HB3	1:B:465:ILE:CG1	2.42	0.47
1:B:366:LYS:HZ3	1:B:448:ILE:HD11	1.79	0.47
1:B:339:LEU:O	1:B:340:ILE:C	2.52	0.47
1:A:173:PHE:O	1:A:176:ILE:HG12	2.14	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:433:PHE:HA	1:B:434:PRO:HD3	1.78	0.46
1:B:248:ASP:HA	1:B:249:PRO:HD2	1.67	0.46
1:B:98:THR:CG2	1:B:98:THR:O	2.64	0.46
1:B:419:MET:HG2	1:B:464:VAL:HG21	1.98	0.46
1:B:512:VAL:O	1:B:513:GLU:C	2.54	0.46
1:A:452:LEU:HD13	1:A:492:LEU:CD2	2.46	0.46
1:B:467:VAL:CG1	1:B:468:CYS:N	2.79	0.45
1:B:433:PHE:CD2	1:B:433:PHE:N	2.84	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: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:327:ASN:HA	1:B:327:ASN:ND2	2.31	0.45
1:B:373:ASP:HA	1:B:381:SER:HB3	1.98	0.45
1:A:388:CYS:O	1:A:390:GLU:N	2.47	0.45
1:A:184:ARG:HH22	1:A:208:ALA:HB2	1.82	0.45
1:B:432:ARG:C	1:B:433:PHE:CD2	2.90	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:520:ASN:N	1:A:520:ASN:ND2	2.60	0.45
1:A:366:LYS:HE2	1:A:387:GLU:OE2	2.16	0.45
1:A:223:LEU:CD1	1:A:230:VAL:CG2	2.95	0.45
1:B:205:PHE:CD2	1:B:205:PHE:N	2.84	0.45
1:A:241:ASN:C	1:A:241:ASN:ND2	2.65	0.44
1:B:458:ASN:HA	1:B:465:ILE:CD1	2.48	0.44
1:B:91:MET:HG2	1:B:94:MET:HB3	2.00	0.44
1:B:380:PHE:HZ	1:B:412:ALA:HB1	1.82	0.44
1:A:101:ILE:CD1	1:A:332:VAL:HG21	2.43	0.44
1:A:388:CYS:C	1:A:390:GLU:N	2.71	0.44
1:B:97:MET:SD	1:B:336:LEU:HD21	2.58	0.44
1:A:351:LEU:CD1	1:A:371:ILE:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:HB2	1:A:484:PHE:CG	2.53	0.44
1:A:246:TYR:CE2	1:A:262:LYS:HE2	2.53	0.44
1:A:269:MET:CE	1:A:303:PHE:CB	2.76	0.44
1:B:380:PHE:CZ	1:B:412:ALA:HB1	2.53	0.44
1:A:213:LEU:HB3	1:A:217:SER:CB	2.47	0.44
1:A:462:ASN:C	1:A:462:ASN:ND2	2.70	0.44
1:A:346:SER:O	1:A:347:LEU:C	2.56	0.44
1:A:127:ASP:HB2	1:B:100:LYS:NZ	2.32	0.44
1:B:486:ARG:HH11	1:B:486:ARG:HG3	1.82	0.44
1:B:303:PHE:O	1:B:307:LEU:HG	2.18	0.44
1:B:419:MET:O	1:B:420:GLU:CG	2.59	0.44
1:A:258:ILE:O	1:A:258:ILE:HG23	2.17	0.44
1:B:384:PHE:HD2	1:B:385:HIS:N	2.15	0.44
1:B:246:TYR:CD2	1:B:262:LYS:NZ	2.86	0.44
1:A:273:ASN:OD1	1:A:273:ASN:C	2.57	0.44
1:B:291:ASN:HD22	1:B:291:ASN:N	2.14	0.43
1:B:450:SER:H	1:B:472:ASN:HD22	1.65	0.43
1:B:423:ASN:HD21	1:B:484:PHE:HB2	1.81	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:427:VAL:HG21	1:B:448:ILE:HG22	2.00	0.43
1:B:294:THR:HG23	1:B:295:PHE:H	1.82	0.43
1:A:351:LEU:HD21	1:A:503:ILE:HD13	2.01	0.43
1:B:230:VAL:O	1:B:231:GLY:C	2.57	0.43
1:B:172:ILE:HD13	1:B:310:CYS:SG	2.59	0.43
1:A:496:VAL:HA	1:A:499:CYS:HB2	2.01	0.43
1:B:368:THR:CG2	1:B:384:PHE:O	2.66	0.43
1:A:118:SER:O	1:A:119:GLU:CB	2.67	0.43
1:B:275:ARG:O	1:B:276:GLU:HB2	2.19	0.43
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:B:481:VAL:HG13	1:B:482:LYS:H	1.84	0.42
1:A:381:SER:OG	1:A:382:SER:N	2.53	0.42
1:B:99:ARG:NE	1:B:99:ARG:HA	2.34	0.42
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.71	0.42
1:A:200:LEU:H	1:A:200:LEU:CD2	2.29	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:B:148:GLN:CA	1:B:148:GLN:NE2	2.68	0.42
1:B:98:THR:HG22	1:B:98:THR:O	2.19	0.42
1:A:336:LEU:O	1:A:340:ILE:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LEU:HD13	1:A:357:THR:HG21	2.01	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:B:368:THR:HG23	1:B:385:HIS:HD2	1.85	0.42
1:A:184:ARG:HB3	1:A:206:ASP:CB	2.49	0.42
1:A:151:ARG:HD2	1:A:151:ARG:HA	1.76	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:B:269:MET:HE3	1:B:303:PHE:CG	2.55	0.41
1:A:184:ARG:NH2	1:A:208:ALA:HB2	2.35	0.41
1:A:460:LYS:HG2	1:A:460:LYS:H	1.47	0.41
1:B:473:LYS:HB3	1:B:482:LYS:O	2.21	0.41
1:A:352:LYS:HB3	1:A:352:LYS:NZ	2.35	0.41
1:B:447:CYS:O	1:B:448:ILE:C	2.59	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:B:103:ALA:CB	1:B:361:PHE:HE2	2.17	0.41
1:A:458:ASN:ND2	1:A:458:ASN:H	2.11	0.41
1:B:478:THR:HG21	1:B:480:LYS:HB2	2.02	0.41
1:B:358:ILE:HG21	1:B:470:LEU:HD21	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:B:180:ILE:HD13	1:B:180:ILE:N	2.35	0.41
1:A:407:ILE:O	1:A:409:TYR:CD2	2.74	0.41
1:A:430:ASP:C	1:A:430:ASP:OD1	2.60	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:464:VAL:O	1:B:465:ILE:C	2.60	0.40
1:B:450:SER:OG	1:B:472:ASN:HA	2.22	0.40
1:B:239:PRO:O	1:B:240:LEU:HD23	2.21	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%)	11	34
1	B	370/431 (86%)	303 (82%)	51 (14%)	16 (4%)	3	10
All	All	753/862 (87%)	638 (85%)	92 (12%)	23 (3%)	5	17

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	VAL
1	A	390	GLU
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%)	299 (86%)	50 (14%)	4	12
1	B	340/387 (88%)	273 (80%)	67 (20%)	1	5
All	All	689/774 (89%)	572 (83%)	117 (17%)	2	7

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ILE
1	A	115	VAL
1	A	119	GLU
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	219	ASN
1	A	223	LEU
1	A	230	VAL
1	A	241	ASN
1	A	242	ILE
1	A	243	LYS
1	A	258	ILE
1	A	264	GLN
1	A	289	SER
1	A	303	PHE
1	A	326	GLU
1	A	328	LYS
1	A	339	LEU
1	A	374	GLU
1	A	377	SER
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	427	VAL

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Mol	Chain	Res	Type
1	A	430	ASP
1	A	447	CYS
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	512	VAL
1	A	519	ARG
1	A	520	ASN
1	B	96	SER
1	B	99	ARG
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	180	ILE
1	B	201	ILE
1	B	203	ARG
1	B	207	VAL
1	B	233	VAL
1	B	236	LEU
1	B	248	ASP
1	B	250	ARG
1	B	252	ASN
1	B	264	GLN
1	B	269	MET
1	B	277	GLU
1	B	291	ASN
1	B	294	THR
1	B	301	LYS
1	B	318	GLN
1	B	338	SER

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Mol	Chain	Res	Type
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	360	SER
1	B	362	MET
1	B	368	THR
1	B	380	PHE
1	B	383	VAL
1	B	387	GLU
1	B	389	GLU
1	B	390	GLU
1	B	391	LEU
1	B	394	SER
1	B	409	TYR
1	B	410	MET
1	B	416	LYS
1	B	418	THR
1	B	429	LYS
1	B	430	ASP
1	B	431	LYS
1	B	432	ARG
1	B	433	PHE
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	476	GLU
1	B	480	LYS
1	B	493	GLU
1	B	504	GLN
1	B	508	MET
1	B	513	GLU
1	B	514	ARG
1	B	516	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	218	ASN
1	A	219	ASN
1	A	241	ASN
1	A	252	ASN
1	A	274	HIS
1	A	283	GLN
1	A	315	HIS
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	252	ASN
1	B	257	GLN
1	B	291	ASN
1	B	315	HIS
1	B	327	ASN
1	B	330	ASN
1	B	345	GLN
1	B	385	HIS
1	B	458	ASN
1	B	472	ASN
1	B	490	GLN
1	B	505	ASN
1	B	520	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	391/431 (90%)	0.01	26 (6%)	22 13	43, 77, 123, 156	0
1	B	380/431 (88%)	0.07	16 (4%)	40 28	48, 83, 132, 181	0
All	All	771/862 (89%)	0.04	42 (5%)	29 19	43, 79, 129, 181	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	ALA	10.3
1	B	129	GLU	7.9
1	A	213	LEU	6.5
1	B	391	LEU	6.4
1	A	212	THR	5.1
1	B	128	SER	5.1
1	A	211	SER	4.9
1	B	91	MET	4.8
1	A	446	GLN	4.7
1	A	391	LEU	4.6
1	B	130	LYS	4.4
1	B	520	ASN	4.3
1	A	291	ASN	4.2
1	B	392	GLU	4.1
1	A	394	SER	4.1
1	A	393	LYS	3.9
1	A	119	GLU	3.8
1	B	92	GLU	3.8
1	B	93	HIS	3.7
1	A	292	GLY	3.5
1	A	118	SER	3.5
1	A	210	GLY	3.3
1	B	394	SER	3.3
1	B	97	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	99	ARG	3.1
1	A	209	GLU	2.8
1	A	392	GLU	2.7
1	A	218	ASN	2.7
1	A	117	ASP	2.6
1	A	520	ASN	2.6
1	A	216	VAL	2.6
1	A	290	GLY	2.5
1	A	499	CYS	2.5
1	B	366	LYS	2.5
1	B	96	SER	2.4
1	A	120	GLY	2.4
1	A	447	CYS	2.4
1	A	453	CYS	2.3
1	A	519	ARG	2.2
1	A	127	ASP	2.2
1	B	433	PHE	2.1
1	A	214	GLU	2.1

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 carbohydrates 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.