



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:05 PM UTC

PDB ID : 4DDQ / pdb_00004ddq
Title : Structural plasticity of the Bacillus subtilis GyrA homodimer
Authors : Rudolph, M.G.; Klostermeier, D.
Deposited on : 2012-01-19
Resolution : 3.30 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

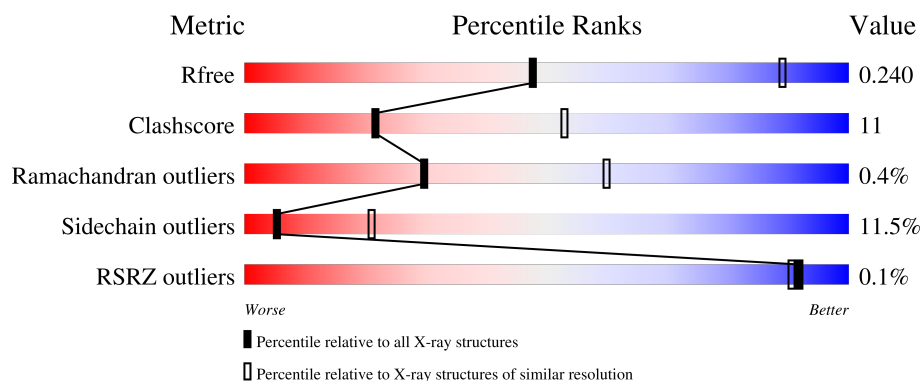
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	502	
1	B	502	
1	C	502	
1	D	502	
1	E	502	

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Mol	Chain	Length	Quality of chain
1	F	502	65% 22% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21664 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 DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3624	2266	650	694	14			
1	B	457	Total	C	N	O	S	0	0	0
			3618	2263	649	692	14			
1	C	455	Total	C	N	O	S	0	0	0
			3606	2255	647	690	14			
1	D	455	Total	C	N	O	S	0	0	0
			3607	2256	647	691	13			
1	E	456	Total	C	N	O	S	0	0	0
			3609	2255	648	692	14			
1	F	452	Total	C	N	O	S	0	0	0
			3583	2241	641	687	14			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		
2	F	1	Total	K	0	0
			1	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			8	4	1	3		

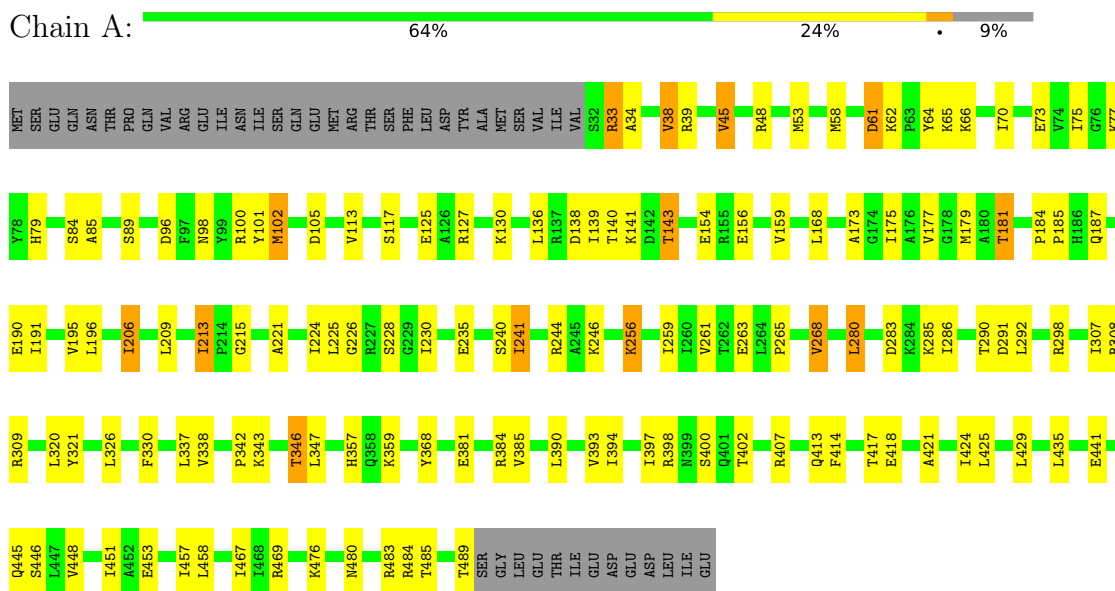
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	D	2	Total	O	0	0
			2	2		

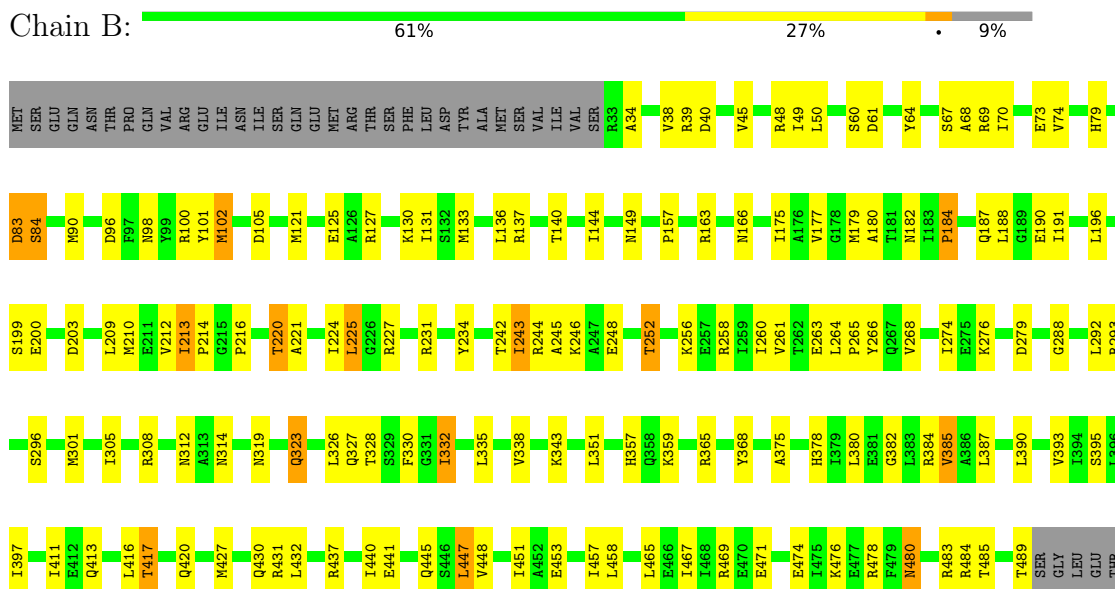
3 Residue-property plots

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: DNA gyrase subunit A



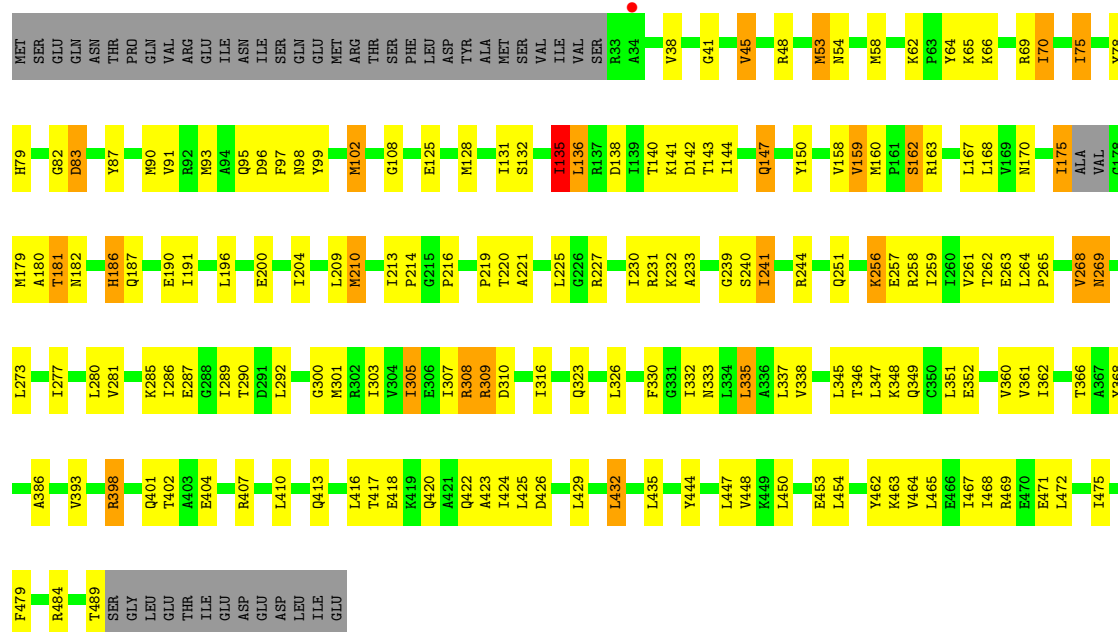
• Molecule 1: DNA gyrase subunit A



ILE
GLU
GLU
ASP
ASP
LEU
ILE
GLU

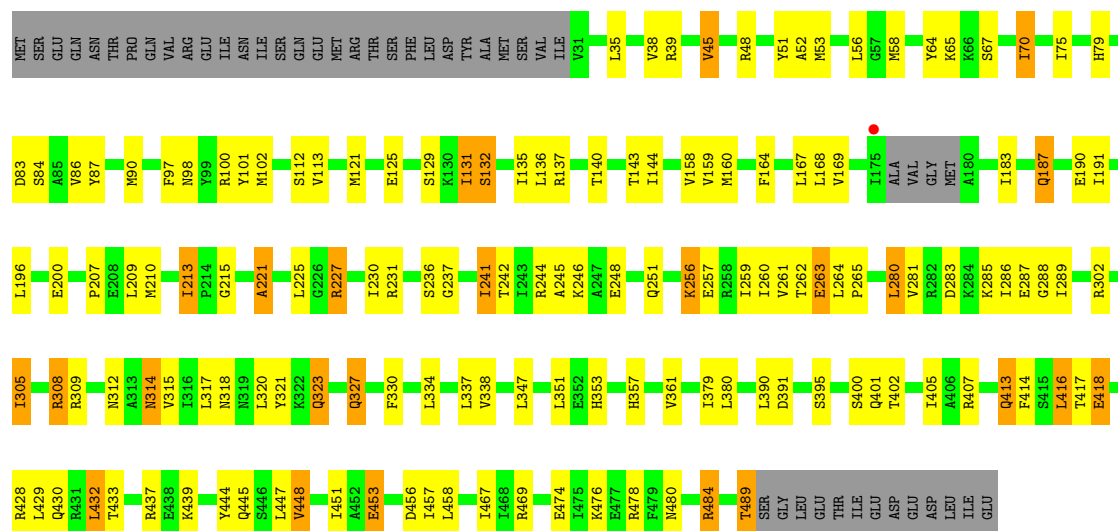
• Molecule 1: DNA gyrase subunit A

Chain C: 56% 29% 5% 9%



• Molecule 1: DNA gyrase subunit A

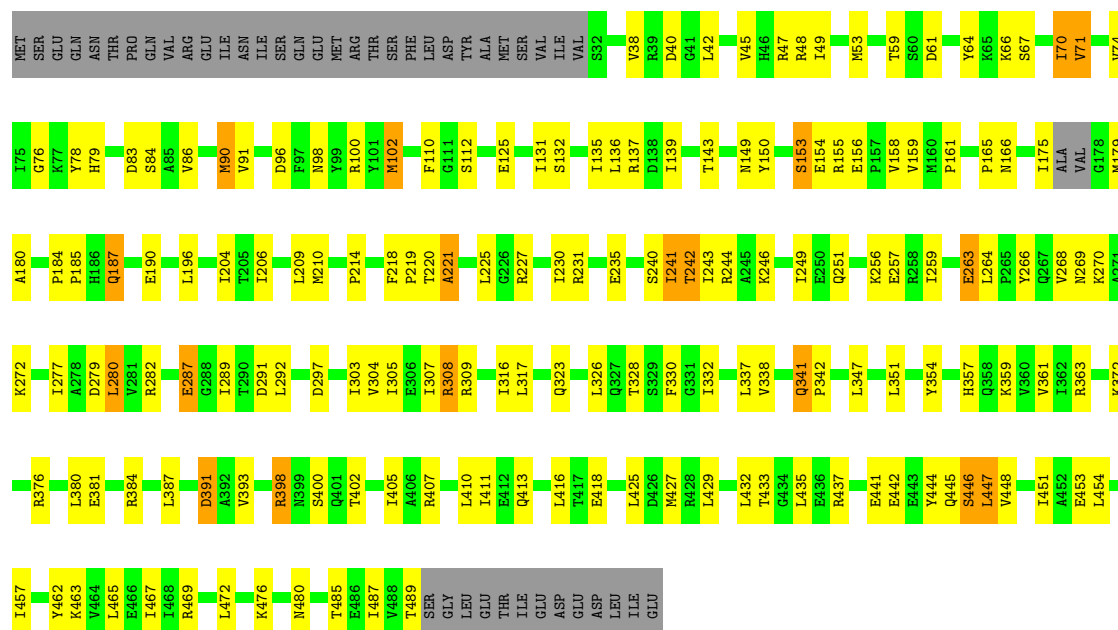
Chain D: 61% 25% 5% 9%



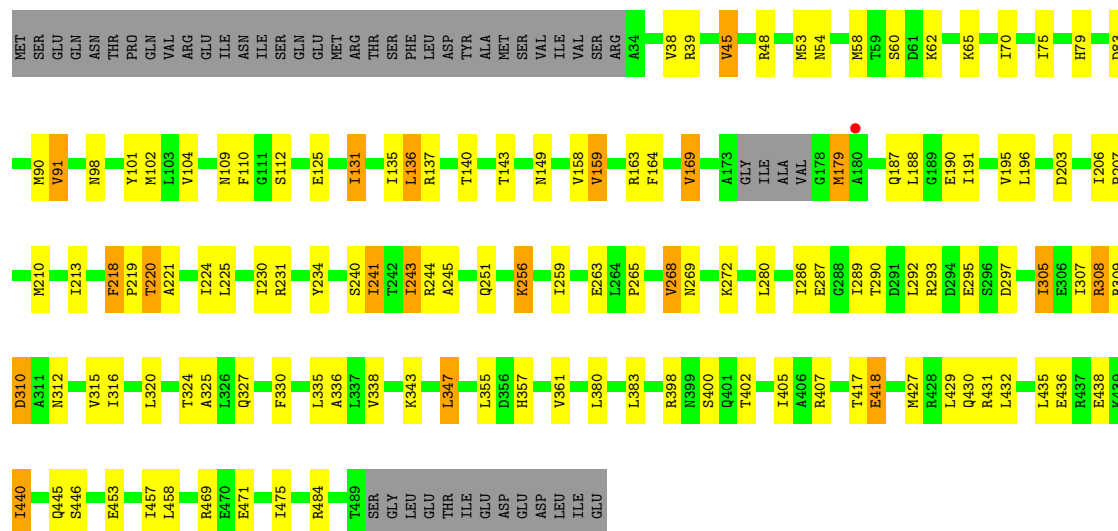
• Molecule 1: DNA gyrase subunit A

Chain E: 57% 30% 9%





- Molecule 1: DNA gyrase subunit A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.80Å 165.11Å 180.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 3.30 49.02 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.02-3.30) 95.1 (49.02-3.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_934)	Depositor
R, R_{free}	0.174 , 0.235 0.179 , 0.240	Depositor DCC
R_{free} test set	3499 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	131.4	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 108.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21664	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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: TRS, K

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	0.57	0/3671	0.95	8/4950 (0.2%)
1	B	0.59	0/3665	1.02	9/4942 (0.2%)
1	C	0.61	0/3652	1.02	13/4922 (0.3%)
1	D	0.54	0/3653	0.94	6/4925 (0.1%)
1	E	0.53	0/3655	0.94	3/4926 (0.1%)
1	F	0.51	0/3629	0.96	7/4892 (0.1%)
All	All	0.56	0/21925	0.97	46/29557 (0.2%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	62	LYS	CA-C-N	7.22	127.27	119.90
1	F	62	LYS	C-N-CA	7.22	127.27	119.90
1	C	285	LYS	N-CA-C	-6.79	105.29	113.97
1	E	150	TYR	N-CA-C	6.70	118.58	111.28
1	F	218	PHE	CA-C-N	6.36	126.05	119.56
1	F	218	PHE	C-N-CA	6.36	126.05	119.56
1	C	45	VAL	CB-CA-C	-6.33	103.86	111.97
1	C	62	LYS	CA-C-N	-6.32	114.26	120.52
1	C	62	LYS	C-N-CA	-6.32	114.26	120.52
1	E	153	SER	N-CA-C	6.28	118.20	111.36
1	B	184	PRO	CA-C-N	6.18	126.15	120.03
1	B	184	PRO	C-N-CA	6.18	126.15	120.03
1	B	177	VAL	N-CA-C	6.09	116.87	110.72
1	A	62	LYS	CA-C-N	6.09	127.45	119.84
1	A	62	LYS	C-N-CA	6.09	127.45	119.84
1	D	418	GLU	N-CA-C	-6.00	104.82	111.36
1	D	213	ILE	CA-C-N	5.97	126.12	119.32
1	D	213	ILE	C-N-CA	5.97	126.12	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	LEU	CA-C-N	-5.86	118.05	122.33
1	B	225	LEU	C-N-CA	-5.86	118.05	122.33
1	B	480	ASN	N-CA-C	5.71	118.04	108.96
1	C	450	LEU	N-CA-C	5.71	117.18	111.07
1	A	206	ILE	CA-C-N	-5.71	112.70	119.84
1	A	206	ILE	C-N-CA	-5.71	112.70	119.84
1	C	300	GLY	N-CA-C	5.68	118.28	110.56
1	F	336	ALA	N-CA-C	5.49	115.49	108.24
1	B	225	LEU	N-CA-C	5.49	118.10	111.40
1	A	184	PRO	CA-C-N	5.35	125.65	119.92
1	A	184	PRO	C-N-CA	5.35	125.65	119.92
1	C	186	HIS	N-CA-C	5.29	117.23	109.24
1	C	360	VAL	N-CA-C	5.23	115.44	110.42
1	F	104	VAL	N-CA-C	5.21	115.47	107.77
1	C	150	TYR	N-CA-C	5.20	117.35	111.11
1	A	213	ILE	CA-C-N	5.18	124.80	119.05
1	A	213	ILE	C-N-CA	5.18	124.80	119.05
1	E	326	LEU	N-CA-C	-5.15	106.95	113.18
1	C	227	ARG	N-CA-C	-5.12	105.78	112.23
1	D	183	ILE	N-CA-C	5.11	112.92	107.76
1	C	179	MET	N-CA-C	5.06	116.64	108.34
1	D	264	LEU	CA-C-N	5.05	124.98	119.78
1	D	264	LEU	C-N-CA	5.05	124.98	119.78
1	C	108	GLY	N-CA-C	-5.04	104.91	111.52
1	C	135	ILE	N-CA-C	-5.02	105.52	111.00
1	F	109	ASN	N-CA-C	5.02	116.82	107.99
1	B	213	ILE	CA-C-N	5.02	125.09	119.87
1	B	213	ILE	C-N-CA	5.02	125.09	119.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3624	0	3705	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3618	0	3700	80	0
1	C	3606	0	3685	101	0
1	D	3607	0	3687	76	0
1	E	3609	0	3681	88	0
1	F	3583	0	3658	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	F	8	0	12	0	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
All	All	21664	0	22128	472	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 (472) 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:F:243:ILE:HD11	1:F:330:PHE:HB2	1.53	0.90
1:E:384:ARG:NH1	1:E:441:GLU:OE2	2.08	0.86
1:A:230:ILE:HG12	1:A:241:ILE:HD11	1.59	0.84
1:B:243:ILE:HD11	1:B:330:PHE:HB2	1.61	0.81
1:B:432:LEU:O	1:B:437:ARG:NH1	2.14	0.80
1:A:58:MET:HE3	1:A:65:LYS:HB2	1.63	0.79
1:C:230:ILE:HG12	1:C:241:ILE:HD11	1.67	0.77
1:A:58:MET:HG2	1:A:65:LYS:HD2	1.66	0.77
1:F:259:ILE:HB	1:F:305:ILE:HG23	1.65	0.76
1:E:230:ILE:HG12	1:E:241:ILE:HD11	1.66	0.76
1:B:225:LEU:HB2	1:B:242:THR:HB	1.67	0.75
1:C:210:MET:HE1	1:C:231:ARG:HG3	1.69	0.75
1:B:210:MET:HE1	1:B:231:ARG:HG3	1.68	0.75
1:C:196:LEU:HD22	1:C:469:ARG:HG2	1.71	0.73
1:D:210:MET:HE1	1:D:231:ARG:HG3	1.72	0.72
1:C:48:ARG:HD3	1:C:79:HIS:HB2	1.72	0.72
1:F:210:MET:HE1	1:F:231:ARG:HG3	1.72	0.72
1:D:237:GLY:HA2	1:D:334:LEU:HD12	1.71	0.71
1:C:261:VAL:HB	1:C:303:ILE:HB	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:ILE:HG12	1:D:241:ILE:HD11	1.72	0.71
1:D:58:MET:HG2	1:D:65:LYS:HD2	1.71	0.71
1:B:48:ARG:HD3	1:B:79:HIS:HB2	1.72	0.70
1:D:241:ILE:HG22	1:D:330:PHE:HB3	1.75	0.69
1:F:196:LEU:HD22	1:F:469:ARG:HG2	1.74	0.69
1:D:38:VAL:HG21	1:D:338:VAL:HG22	1.75	0.69
1:B:457:ILE:HD13	1:B:467:ILE:HD11	1.73	0.68
1:C:96:ASP:HA	1:C:102:MET:HE2	1.74	0.68
1:F:312:ASN:HB2	1:F:315:VAL:HG23	1.75	0.68
1:C:45:VAL:HG22	1:C:79:HIS:CE1	2.29	0.67
1:F:225:LEU:HD11	1:F:244:ARG:HD3	1.75	0.67
1:F:230:ILE:HG12	1:F:241:ILE:HD11	1.75	0.67
1:A:224:ILE:HG21	1:A:230:ILE:HD11	1.77	0.67
1:C:220:THR:O	1:C:220:THR:OG1	2.13	0.67
1:D:209:LEU:HD21	1:D:351:LEU:HD12	1.75	0.66
1:F:58:MET:HG2	1:F:65:LYS:HD2	1.78	0.65
1:D:256:LYS:HE3	1:D:309:ARG:HH12	1.60	0.65
1:E:143:THR:HB	1:E:361:VAL:HG13	1.77	0.65
1:C:265:PRO:HG2	1:C:268:VAL:HG11	1.78	0.65
1:C:38:VAL:HG21	1:C:338:VAL:HG22	1.76	0.65
1:A:102:MET:HE3	1:A:102:MET:H	1.62	0.65
1:B:191:ILE:HD13	1:B:213:ILE:HD13	1.78	0.65
1:F:307:ILE:HG12	1:F:316:ILE:HD12	1.79	0.65
1:C:281:VAL:HG21	1:C:289:ILE:HB	1.79	0.65
1:E:225:LEU:HB2	1:E:242:THR:HB	1.78	0.64
1:F:164:PHE:HE2	1:F:169:VAL:HG11	1.62	0.64
1:A:190:GLU:OE1	1:A:483:ARG:NH2	2.29	0.64
1:C:425:LEU:HB3	1:D:430:GLN:HB3	1.79	0.64
1:A:384:ARG:NH1	1:A:441:GLU:OE2	2.32	0.63
1:D:75:ILE:HG13	1:D:86:VAL:HG21	1.79	0.63
1:B:100:ARG:HG3	1:B:101:TYR:CE2	2.33	0.63
1:F:179:MET:HB2	1:F:335:LEU:HD21	1.80	0.63
1:B:382:GLY:HA3	1:B:420:GLN:HG2	1.81	0.62
1:F:407:ARG:HD2	1:F:418:GLU:OE1	1.99	0.62
1:C:147:GLN:NE2	1:F:125:GLU:OE1	2.32	0.62
1:D:100:ARG:NH1	1:D:484:ARG:HD3	2.15	0.62
1:E:206:ILE:HG21	1:E:235:GLU:HG3	1.81	0.62
1:C:259:ILE:HG13	1:C:307:ILE:HD11	1.82	0.62
1:F:224:ILE:HG21	1:F:230:ILE:HD11	1.82	0.62
1:B:474:GLU:OE2	1:B:478:ARG:NE	2.30	0.61
1:D:48:ARG:HD3	1:D:79:HIS:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:THR:O	1:B:220:THR:OG1	2.18	0.61
1:E:204:ILE:HD13	1:E:209:LEU:HD13	1.81	0.61
1:F:158:VAL:HG23	1:F:159:VAL:HG22	1.82	0.61
1:B:196:LEU:HD22	1:B:469:ARG:HG2	1.83	0.60
1:D:314:ASN:O	1:D:318:ASN:ND2	2.33	0.60
1:F:245:ALA:HB2	1:F:265:PRO:HD3	1.82	0.60
1:A:246:LYS:HB3	1:A:263:GLU:HB2	1.83	0.60
1:B:137:ARG:HB3	1:B:163:ARG:HG3	1.82	0.60
1:F:320:LEU:O	1:F:324:THR:OG1	2.19	0.60
1:E:457:ILE:HD13	1:E:467:ILE:HD11	1.83	0.59
1:C:292:LEU:HD12	1:C:305:ILE:HB	1.85	0.59
1:F:269:ASN:HB3	1:F:272:LYS:HB2	1.85	0.59
1:C:187:GLN:HG3	1:C:190:GLU:H	1.68	0.58
1:E:376:ARG:HB3	1:E:447:LEU:HD21	1.84	0.58
1:A:38:VAL:HG21	1:A:338:VAL:HG22	1.85	0.58
1:E:297:ASP:OD1	1:E:297:ASP:N	2.36	0.58
1:F:195:VAL:HG12	1:F:355:LEU:HD13	1.86	0.58
1:A:196:LEU:HD22	1:A:469:ARG:HG2	1.85	0.58
1:B:144:ILE:HD13	1:B:157:PRO:HB3	1.86	0.57
1:E:40:ASP:CG	1:E:42:LEU:HD12	2.28	0.57
1:E:269:ASN:HB3	1:E:272:LYS:HB2	1.85	0.57
1:C:38:VAL:HG23	1:C:337:LEU:O	2.04	0.57
1:B:179:MET:HB3	1:B:335:LEU:HD21	1.86	0.57
1:C:345:LEU:HB3	1:C:349:GLN:HB2	1.86	0.57
1:B:105:ASP:HB3	1:B:127:ARG:HG3	1.86	0.57
1:D:38:VAL:HA	1:D:167:LEU:HD22	1.87	0.57
1:A:100:ARG:HB2	1:A:185:PRO:HB3	1.87	0.57
1:D:100:ARG:HG3	1:D:101:TYR:CE2	2.40	0.57
1:E:251:GLN:HE21	1:E:257:GLU:HG2	1.69	0.56
1:C:99:TYR:HD1	1:C:170:ASN:CG	2.12	0.56
1:E:221:ALA:HB3	1:E:263:GLU:HG2	1.87	0.56
1:A:100:ARG:HG3	1:A:101:TYR:CE2	2.40	0.56
1:C:64:TYR:HB3	1:C:125:GLU:HB3	1.87	0.56
1:E:187:GLN:HG3	1:E:190:GLU:H	1.68	0.56
1:E:220:THR:O	1:E:220:THR:OG1	2.18	0.56
1:F:39:ARG:NE	1:F:159:VAL:HG11	2.19	0.56
1:B:39:ARG:HB3	1:B:357:HIS:CG	2.40	0.56
1:F:206:ILE:HG22	1:F:210:MET:HE2	1.86	0.56
1:F:256:LYS:HE3	1:F:309:ARG:HH22	1.71	0.56
1:E:48:ARG:HD3	1:E:79:HIS:HB2	1.87	0.56
1:E:359:LYS:HE2	1:E:465:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:ARG:HD2	1:E:418:GLU:OE1	2.05	0.56
1:B:39:ARG:HB3	1:B:357:HIS:CD2	2.41	0.55
1:E:196:LEU:HD22	1:E:469:ARG:HG2	1.89	0.55
1:C:136:LEU:HD11	1:C:160:MET:HE3	1.89	0.55
1:F:292:LEU:HD12	1:F:305:ILE:HB	1.89	0.55
1:A:102:MET:H	1:A:102:MET:CE	2.19	0.55
1:B:387:LEU:HD23	1:B:390:LEU:HD13	1.88	0.55
1:D:259:ILE:HB	1:D:305:ILE:HG23	1.89	0.55
1:C:69:ARG:HA	1:E:76:GLY:HA2	1.89	0.55
1:A:298:ARG:HE	1:D:353:HIS:CD2	2.25	0.54
1:C:386:ALA:HB2	1:C:424:ILE:HG12	1.88	0.54
1:C:221:ALA:HB3	1:C:263:GLU:HG2	1.89	0.54
1:E:256:LYS:HE3	1:E:309:ARG:HH22	1.70	0.54
1:B:227:ARG:HG3	1:B:489:THR:HG23	1.90	0.54
1:B:245:ALA:HB2	1:B:265:PRO:HD3	1.88	0.54
1:B:296:SER:HB3	1:B:301:MET:HA	1.89	0.54
1:A:244:ARG:HD2	1:A:321:TYR:CE2	2.43	0.54
1:B:175:ILE:HG12	1:B:180:ALA:HB1	1.89	0.54
1:E:38:VAL:HG21	1:E:338:VAL:HG22	1.89	0.54
1:E:393:VAL:HG13	1:E:410:LEU:HD21	1.88	0.54
1:A:105:ASP:HB3	1:A:127:ARG:HG3	1.90	0.54
1:F:338:VAL:HB	1:F:343:LYS:HD3	1.89	0.54
1:D:45:VAL:HG22	1:D:79:HIS:CE1	2.43	0.54
1:F:191:ILE:O	1:F:195:VAL:HG23	2.08	0.53
1:B:393:VAL:O	1:B:397:ILE:HG13	2.07	0.53
1:C:265:PRO:HG2	1:C:268:VAL:CG1	2.39	0.53
1:F:427:MET:HE2	1:F:431:ARG:HB3	1.91	0.53
1:A:393:VAL:O	1:A:397:ILE:HG13	2.08	0.53
1:F:91:VAL:HG22	1:F:110:PHE:CD2	2.43	0.53
1:C:265:PRO:O	1:C:268:VAL:HG13	2.09	0.53
1:F:218:PHE:HE2	1:F:224:ILE:HD11	1.74	0.53
1:D:207:PRO:HA	1:D:210:MET:HE3	1.91	0.53
1:D:453:GLU:O	1:D:457:ILE:HG13	2.08	0.53
1:F:290:THR:OG1	1:F:308:ARG:HG3	2.09	0.53
1:D:457:ILE:HD13	1:D:467:ILE:HD11	1.91	0.52
1:C:241:ILE:HG22	1:C:330:PHE:HB3	1.91	0.52
1:D:129:SER:OG	1:D:132:SER:HB3	2.10	0.52
1:E:38:VAL:HG23	1:E:337:LEU:O	2.09	0.52
1:A:407:ARG:HD2	1:A:418:GLU:OE1	2.09	0.52
1:E:209:LEU:HD21	1:E:351:LEU:HD12	1.90	0.52
1:A:141:LYS:HG2	1:A:368:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:VAL:HA	1:C:467:ILE:HD12	1.92	0.52
1:A:33:ARG:HH21	1:A:342:PRO:HD3	1.75	0.52
1:C:135:ILE:HG22	1:C:136:LEU:HD12	1.91	0.52
1:A:280:LEU:HD13	1:A:285:LYS:HB2	1.91	0.52
1:E:214:PRO:HB2	1:E:487:ILE:HD12	1.92	0.52
1:C:58:MET:O	1:C:128:MET:HG3	2.10	0.52
1:C:256:LYS:HE3	1:C:309:ARG:HH22	1.75	0.52
1:C:259:ILE:HB	1:C:305:ILE:HG23	1.91	0.52
1:E:210:MET:HE1	1:E:231:ARG:HG3	1.91	0.52
1:C:230:ILE:CG1	1:C:241:ILE:HD11	2.38	0.52
1:D:53:MET:HG2	1:D:58:MET:HE2	1.92	0.51
1:E:230:ILE:CG1	1:E:241:ILE:HD11	2.39	0.51
1:A:265:PRO:HD2	1:A:268:VAL:HG21	1.92	0.51
1:B:384:ARG:NH1	1:B:441:GLU:OE2	2.33	0.51
1:C:209:LEU:HD21	1:C:351:LEU:HD12	1.92	0.51
1:A:61:ASP:OD1	1:A:61:ASP:N	2.31	0.51
1:B:265:PRO:O	1:B:268:VAL:HG13	2.10	0.51
1:A:168:LEU:HD13	1:A:191:ILE:HD12	1.91	0.51
1:D:221:ALA:HB3	1:D:263:GLU:HG2	1.92	0.51
1:A:457:ILE:HD13	1:A:467:ILE:HD11	1.93	0.51
1:D:433:THR:O	1:D:437:ARG:HG3	2.11	0.51
1:E:391:ASP:OD2	1:E:391:ASP:N	2.43	0.51
1:B:359:LYS:HE2	1:B:465:LEU:HD21	1.91	0.51
1:E:270:LYS:HD2	1:E:303:ILE:HD11	1.93	0.51
1:F:207:PRO:HA	1:F:210:MET:HE3	1.93	0.50
1:A:39:ARG:HB3	1:A:357:HIS:CG	2.46	0.50
1:A:190:GLU:CD	1:A:483:ARG:HH21	2.14	0.50
1:C:53:MET:HG3	1:C:70:ILE:HD13	1.93	0.50
1:E:53:MET:HG3	1:E:70:ILE:HD13	1.94	0.50
1:D:196:LEU:HD22	1:D:469:ARG:HG2	1.93	0.50
1:B:288:GLY:HA2	1:B:308:ARG:HD3	1.94	0.50
1:D:245:ALA:HB2	1:D:265:PRO:HD3	1.92	0.50
1:B:38:VAL:HG21	1:B:338:VAL:HG22	1.94	0.50
1:A:45:VAL:HG22	1:A:79:HIS:CE1	2.47	0.50
1:A:96:ASP:HA	1:A:102:MET:SD	2.51	0.50
1:C:138:ASP:O	1:C:143:THR:OG1	2.26	0.49
1:F:48:ARG:HD3	1:F:79:HIS:HB2	1.94	0.49
1:C:83:ASP:HB3	1:E:83:ASP:H	1.77	0.49
1:E:64:TYR:HB3	1:E:125:GLU:HB3	1.94	0.49
1:C:232:LYS:HE2	1:C:239:GLY:HA2	1.95	0.49
1:A:283:ASP:HB3	1:A:285:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:MET:HG3	1:B:431:ARG:HD3	1.94	0.49
1:C:175:ILE:HA	1:C:180:ALA:HB2	1.93	0.49
1:C:264:LEU:H	1:C:301:MET:HE1	1.77	0.49
1:E:448:VAL:O	1:E:451:ILE:HG13	2.12	0.49
1:F:54:ASN:CG	1:F:136:LEU:HD22	2.37	0.49
1:F:380:LEU:HA	1:F:383:LEU:HD12	1.93	0.49
1:C:200:GLU:HG3	1:C:469:ARG:HH21	1.78	0.49
1:C:420:GLN:O	1:C:423:ALA:HB3	2.13	0.49
1:D:400:SER:HB3	1:D:405:ILE:HG22	1.93	0.49
1:E:71:VAL:HG22	1:E:86:VAL:HG12	1.95	0.49
1:D:64:TYR:HB3	1:D:125:GLU:HB3	1.94	0.49
1:E:40:ASP:OD2	1:E:47:ARG:HD3	2.13	0.49
1:F:39:ARG:HB3	1:F:357:HIS:CD2	2.47	0.49
1:A:290:THR:OG1	1:A:308:ARG:HG3	2.12	0.49
1:C:83:ASP:H	1:E:83:ASP:HB3	1.78	0.49
1:A:425:LEU:HB3	1:B:430:GLN:HB3	1.94	0.48
1:A:138:ASP:O	1:A:143:THR:OG1	2.23	0.48
1:D:143:THR:HB	1:D:361:VAL:HG13	1.95	0.48
1:E:357:HIS:O	1:E:361:VAL:HG23	2.12	0.48
1:E:442:GLU:O	1:E:446:SER:HB2	2.13	0.48
1:B:212:VAL:O	1:B:214:PRO:HD3	2.14	0.48
1:D:474:GLU:OE2	1:D:478:ARG:NE	2.42	0.48
1:F:38:VAL:HG21	1:F:338:VAL:HG22	1.95	0.48
1:A:38:VAL:HG23	1:A:337:LEU:O	2.14	0.48
1:A:413:GLN:HB3	1:A:414:PHE:CD2	2.47	0.48
1:A:421:ALA:HA	1:A:424:ILE:HD12	1.94	0.48
1:C:41:GLY:CA	1:C:167:LEU:HB2	2.44	0.48
1:D:244:ARG:HD2	1:D:321:TYR:CE2	2.49	0.48
1:D:281:VAL:HG21	1:D:289:ILE:HB	1.96	0.48
1:B:476:LYS:O	1:B:480:ASN:HB2	2.13	0.48
1:F:289:ILE:HD13	1:F:305:ILE:HD11	1.96	0.48
1:B:384:ARG:HD2	1:B:441:GLU:OE2	2.14	0.48
1:B:447:LEU:O	1:B:451:ILE:HG23	2.14	0.48
1:D:227:ARG:HG3	1:D:489:THR:OG1	2.14	0.48
1:A:221:ALA:HB2	1:A:484:ARG:HB3	1.95	0.48
1:A:320:LEU:HB3	1:A:326:LEU:HD12	1.96	0.48
1:D:187:GLN:HG3	1:D:190:GLU:H	1.79	0.48
1:D:317:LEU:HA	1:D:320:LEU:HD12	1.96	0.48
1:E:277:ILE:HA	1:E:280:LEU:HB2	1.95	0.48
1:E:292:LEU:HA	1:E:304:VAL:O	2.14	0.48
1:E:411:ILE:HG23	1:E:416:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:THR:HB	1:F:361:VAL:HG13	1.95	0.48
1:D:260:ILE:HD13	1:D:302:ARG:NH1	2.28	0.47
1:C:181:THR:OG1	1:C:335:LEU:O	2.32	0.47
1:D:51:TYR:HB2	1:D:160:MET:HE1	1.96	0.47
1:A:187:GLN:HG3	1:A:190:GLU:H	1.80	0.47
1:B:96:ASP:OD1	1:B:96:ASP:N	2.45	0.47
1:B:96:ASP:HA	1:B:102:MET:HE2	1.96	0.47
1:E:49:ILE:HG12	1:E:74:VAL:HG21	1.95	0.47
1:F:219:PRO:HA	1:F:484:ARG:HH11	1.79	0.47
1:F:213:ILE:HD12	1:F:347:LEU:HD11	1.95	0.47
1:C:241:ILE:HD12	1:C:332:ILE:HD11	1.95	0.47
1:C:462:TYR:CE1	1:C:463:LYS:HG2	2.49	0.47
1:D:246:LYS:HB3	1:D:263:GLU:HB2	1.95	0.47
1:F:221:ALA:O	1:F:263:GLU:HB3	2.15	0.47
1:C:168:LEU:HD23	1:C:168:LEU:HA	1.62	0.47
1:C:168:LEU:HD13	1:C:191:ILE:HD12	1.96	0.47
1:C:175:ILE:HA	1:C:180:ALA:CB	2.45	0.47
1:C:269:ASN:HD22	1:C:269:ASN:C	2.22	0.47
1:E:398:ARG:HA	1:F:432:LEU:O	2.15	0.47
1:A:476:LYS:O	1:A:480:ASN:HB2	2.14	0.47
1:D:429:LEU:O	1:D:432:LEU:HB2	2.14	0.47
1:B:49:ILE:HA	1:B:74:VAL:HG21	1.97	0.47
1:C:362:ILE:O	1:C:366:THR:HG23	2.15	0.47
1:C:393:VAL:HG13	1:C:410:LEU:HD21	1.96	0.47
1:C:426:ASP:O	1:D:428:ARG:HD3	2.15	0.47
1:E:91:VAL:HG13	1:E:110:PHE:HD2	1.79	0.47
1:E:279:ASP:OD2	1:E:282:ARG:NH2	2.40	0.47
1:C:162:SER:O	1:C:162:SER:OG	2.30	0.47
1:D:225:LEU:HB2	1:D:242:THR:HB	1.96	0.47
1:E:433:THR:O	1:E:437:ARG:HG3	2.15	0.47
1:F:164:PHE:HB3	1:F:475:ILE:HD13	1.97	0.46
1:E:218:PHE:CD1	1:E:266:TYR:HB2	2.50	0.46
1:A:64:TYR:HB3	1:A:125:GLU:HB3	1.98	0.46
1:B:196:LEU:O	1:B:199:SER:HB3	2.16	0.46
1:B:246:LYS:HB3	1:B:263:GLU:HB2	1.95	0.46
1:D:439:LYS:HD2	1:F:438:GLU:OE2	2.15	0.46
1:F:293:ARG:NH2	1:F:295:GLU:OE2	2.47	0.46
1:C:186:HIS:CD2	1:C:216:PRO:HA	2.49	0.46
1:E:40:ASP:O	1:E:166:ASN:HB3	2.15	0.46
1:A:381:GLU:O	1:A:385:VAL:HG23	2.15	0.46
1:C:225:LEU:HD11	1:C:244:ARG:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:TYR:O	1:D:448:VAL:HG23	2.15	0.46
1:E:132:SER:O	1:E:135:ILE:N	2.48	0.46
1:A:48:ARG:NE	1:A:156:GLU:OE2	2.35	0.46
1:B:312:ASN:OD1	1:B:314:ASN:HB2	2.16	0.46
1:C:407:ARG:NE	1:C:422:GLN:OE1	2.48	0.46
1:E:289:ILE:HD13	1:E:305:ILE:HD11	1.97	0.46
1:E:246:LYS:HB3	1:E:263:GLU:HB2	1.98	0.46
1:A:45:VAL:HG13	1:A:79:HIS:CD2	2.50	0.46
1:A:241:ILE:HG22	1:A:330:PHE:HB3	1.97	0.46
1:B:221:ALA:HB2	1:B:484:ARG:HB3	1.98	0.46
1:E:175:ILE:HG12	1:E:180:ALA:HB1	1.98	0.46
1:B:130:LYS:O	1:B:133:MET:HB2	2.16	0.45
1:C:58:MET:HG2	1:C:65:LYS:HD2	1.97	0.45
1:C:132:SER:O	1:C:135:ILE:N	2.45	0.45
1:D:407:ARG:HD2	1:D:418:GLU:OE1	2.17	0.45
1:D:448:VAL:O	1:D:451:ILE:HG13	2.16	0.45
1:A:225:LEU:HA	1:A:225:LEU:HD23	1.67	0.45
1:A:280:LEU:HD22	1:A:280:LEU:HA	1.80	0.45
1:F:45:VAL:HG13	1:F:79:HIS:CD2	2.51	0.45
1:A:77:LYS:HG2	1:A:154:GLU:HG3	1.98	0.45
1:B:384:ARG:HH11	1:B:441:GLU:CD	2.22	0.45
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.84	0.45
1:B:64:TYR:HB3	1:B:125:GLU:HB3	1.98	0.45
1:C:465:LEU:HD23	1:C:465:LEU:HA	1.78	0.45
1:D:280:LEU:HD11	1:D:323:GLN:HG2	1.99	0.45
1:B:83:ASP:HB3	1:D:83:ASP:H	1.81	0.45
1:C:143:THR:HB	1:C:361:VAL:HG13	1.97	0.45
1:C:290:THR:OG1	1:C:308:ARG:HG3	2.16	0.45
1:C:187:GLN:HB3	1:C:190:GLU:OE1	2.17	0.45
1:B:276:LYS:O	1:B:279:ASP:HB3	2.17	0.45
1:E:100:ARG:HA	1:E:219:PRO:HB3	1.98	0.45
1:E:206:ILE:HG22	1:E:210:MET:HE2	1.99	0.45
1:F:400:SER:HB3	1:F:405:ILE:HG22	1.98	0.45
1:C:233:ALA:HB1	1:C:332:ILE:HG21	1.99	0.45
1:C:467:ILE:O	1:C:471:GLU:HG3	2.17	0.45
1:F:256:LYS:HE3	1:F:309:ARG:NH2	2.32	0.45
1:A:39:ARG:HB3	1:A:357:HIS:CD2	2.51	0.45
1:D:414:PHE:HB2	1:D:416:LEU:HD11	1.99	0.45
1:A:256:LYS:HE3	1:A:309:ARG:HH12	1.83	0.44
1:A:397:ILE:O	1:A:400:SER:HB2	2.17	0.44
1:D:135:ILE:HG13	1:D:164:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:PRO:HB3	1:E:361:VAL:HG11	1.98	0.44
1:E:241:ILE:HD12	1:E:332:ILE:HD11	1.99	0.44
1:F:101:TYR:CE2	1:F:188:LEU:HB2	2.52	0.44
1:B:209:LEU:HD12	1:B:209:LEU:HA	1.76	0.44
1:B:244:ARG:HG3	1:B:327:GLN:HB2	1.99	0.44
1:C:87:TYR:O	1:C:91:VAL:HG23	2.18	0.44
1:C:219:PRO:HA	1:C:484:ARG:HH11	1.82	0.44
1:A:191:ILE:HD13	1:A:213:ILE:HD13	2.00	0.44
1:C:251:GLN:HE21	1:C:257:GLU:HG2	1.81	0.44
1:C:429:LEU:O	1:C:432:LEU:HB2	2.17	0.44
1:F:245:ALA:HB1	1:F:263:GLU:O	2.17	0.44
1:A:173:ALA:HA	1:A:181:THR:O	2.18	0.44
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.79	0.44
1:B:61:ASP:OD1	1:B:61:ASP:N	2.36	0.44
1:B:264:LEU:HG	1:B:301:MET:HE1	1.99	0.44
1:C:41:GLY:HA3	1:C:167:LEU:HB2	1.98	0.44
1:E:381:GLU:HG3	1:E:444:TYR:HE1	1.82	0.44
1:B:380:LEU:HA	1:B:380:LEU:HD23	1.77	0.44
1:E:184:PRO:HA	1:E:185:PRO:HD3	1.83	0.44
1:F:187:GLN:HG2	1:F:190:GLU:HG3	1.99	0.44
1:B:319:ASN:O	1:B:323:GLN:HB2	2.18	0.44
1:A:206:ILE:HG21	1:A:235:GLU:HG3	1.99	0.44
1:B:292:LEU:HD13	1:B:305:ILE:HG12	1.99	0.44
1:F:308:ARG:HB2	1:F:310:ASP:OD1	2.17	0.44
1:B:67:SER:HB3	1:B:90:MET:HE1	2.00	0.44
1:C:142:ASP:O	1:C:142:ASP:CG	2.61	0.44
1:C:256:LYS:HE3	1:C:309:ARG:NH2	2.32	0.44
1:E:307:ILE:HG22	1:E:308:ARG:O	2.17	0.44
1:A:390:LEU:O	1:A:394:ILE:HG12	2.18	0.43
1:C:91:VAL:O	1:C:95:GLN:HG3	2.17	0.43
1:D:39:ARG:HB3	1:D:357:HIS:CD2	2.53	0.43
1:B:209:LEU:HD21	1:B:351:LEU:HD12	2.01	0.43
1:B:252:THR:HG23	1:B:256:LYS:O	2.18	0.43
1:D:200:GLU:HG3	1:D:469:ARG:HH21	1.82	0.43
1:F:234:TYR:HB3	1:F:347:LEU:HB2	2.00	0.43
1:A:221:ALA:HB1	1:A:484:ARG:O	2.18	0.43
1:C:163:ARG:NH1	1:C:362:ILE:HD11	2.33	0.43
1:D:244:ARG:HG3	1:D:327:GLN:HG3	2.00	0.43
1:E:102:MET:HE3	1:E:102:MET:N	2.33	0.43
1:E:400:SER:HB3	1:E:405:ILE:HG22	2.00	0.43
1:F:436:GLU:O	1:F:440:ILE:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASP:OD1	1:A:292:LEU:N	2.51	0.43
1:C:141:LYS:HB3	1:C:368:TYR:CD2	2.53	0.43
1:E:425:LEU:HD22	1:F:430:GLN:HB3	1.99	0.43
1:F:39:ARG:HD2	1:F:357:HIS:ND1	2.33	0.43
1:F:324:THR:HB	1:F:325:ALA:H	1.62	0.43
1:B:64:TYR:CE1	1:B:127:ARG:HG2	2.54	0.43
1:B:216:PRO:HD3	1:B:234:TYR:OH	2.18	0.43
1:C:273:LEU:HD21	1:C:326:LEU:HG	1.99	0.43
1:E:472:LEU:HA	1:E:472:LEU:HD23	1.76	0.43
1:A:64:TYR:CD1	1:A:127:ARG:HG2	2.54	0.43
1:A:84:SER:OG	1:A:85:ALA:N	2.51	0.43
1:A:343:LYS:HB3	1:A:343:LYS:HE2	1.92	0.43
1:B:380:LEU:HD22	1:B:440:ILE:HG23	1.99	0.43
1:B:385:VAL:HG11	1:B:416:LEU:HD21	2.01	0.43
1:C:213:ILE:HA	1:C:214:PRO:HD3	1.88	0.43
1:C:475:ILE:HG23	1:C:479:PHE:HD2	1.84	0.43
1:D:87:TYR:CD1	1:D:121:MET:HB3	2.54	0.43
1:B:190:GLU:CD	1:B:483:ARG:HH21	2.26	0.43
1:C:444:TYR:O	1:C:448:VAL:HG23	2.18	0.43
1:D:131:ILE:O	1:D:131:ILE:HG13	2.18	0.43
1:E:45:VAL:HG22	1:E:79:HIS:CE1	2.53	0.43
1:F:135:ILE:HG13	1:F:164:PHE:HE1	1.83	0.43
1:B:225:LEU:HD23	1:B:225:LEU:HA	1.48	0.43
1:C:75:ILE:HD11	1:C:82:GLY:C	2.44	0.43
1:C:136:LEU:HD21	1:C:160:MET:HE1	2.01	0.43
1:D:135:ILE:HG13	1:D:164:PHE:CE1	2.54	0.43
1:F:297:ASP:OD1	1:F:297:ASP:N	2.52	0.43
1:A:53:MET:HE3	1:A:70:ILE:HG12	2.01	0.42
1:D:379:ILE:HD13	1:D:379:ILE:HA	1.78	0.42
1:F:244:ARG:HG3	1:F:327:GLN:HG3	2.01	0.42
1:D:97:PHE:CG	1:D:113:VAL:HG22	2.54	0.42
1:E:259:ILE:HB	1:E:305:ILE:HG23	2.01	0.42
1:E:476:LYS:O	1:E:480:ASN:HB2	2.19	0.42
1:F:164:PHE:CE2	1:F:169:VAL:HG11	2.50	0.42
1:A:265:PRO:O	1:A:268:VAL:HG22	2.18	0.42
1:B:224:ILE:HG13	1:B:485:THR:HG21	2.01	0.42
1:B:417:THR:HB	1:B:420:GLN:H	1.84	0.42
1:D:251:GLN:HE21	1:D:257:GLU:CG	2.32	0.42
1:D:380:LEU:HD23	1:D:380:LEU:HA	1.87	0.42
1:F:224:ILE:HD13	1:F:241:ILE:HD13	2.01	0.42
1:F:286:ILE:HD13	1:F:286:ILE:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:429:LEU:HA	1:F:429:LEU:HD23	1.68	0.42
1:C:48:ARG:HG2	1:C:78:TYR:HB3	2.02	0.42
1:E:243:ILE:HD11	1:E:330:PHE:HB2	2.02	0.42
1:E:341:GLN:HA	1:E:342:PRO:HD3	1.78	0.42
1:B:83:ASP:HB2	1:B:121:MET:HE1	2.01	0.42
1:C:286:ILE:HD13	1:C:286:ILE:HA	1.88	0.42
1:B:40:ASP:O	1:B:166:ASN:HB3	2.18	0.42
1:C:398:ARG:NH2	1:D:390:LEU:HB3	2.34	0.42
1:F:427:MET:HG3	1:F:431:ARG:HD3	2.01	0.42
1:D:286:ILE:HD13	1:D:286:ILE:HA	1.78	0.42
1:E:249:ILE:HD11	1:E:317:LEU:HD22	2.01	0.42
1:E:287:GLU:H	1:E:287:GLU:HG2	1.72	0.42
1:D:215:GLY:HA3	1:D:230:ILE:HD13	2.02	0.42
1:E:67:SER:HB3	1:E:90:MET:HE1	2.02	0.42
1:E:165:PRO:HA	1:E:354:TYR:CE1	2.55	0.42
1:A:259:ILE:HG13	1:A:307:ILE:HD11	2.02	0.41
1:B:448:VAL:O	1:B:451:ILE:HG13	2.20	0.41
1:B:184:PRO:HG3	1:B:332:ILE:HD13	2.01	0.41
1:C:256:LYS:HB2	1:C:309:ARG:HH12	1.85	0.41
1:E:264:LEU:HD23	1:E:264:LEU:HA	1.74	0.41
1:E:462:TYR:CE1	1:E:463:LYS:HG2	2.56	0.41
1:F:220:THR:O	1:F:220:THR:OG1	2.38	0.41
1:B:375:ALA:O	1:B:378:HIS:HB3	2.21	0.41
1:C:348:LYS:O	1:C:352:GLU:HG2	2.20	0.41
1:D:52:ALA:O	1:D:56:LEU:HG	2.20	0.41
1:B:175:ILE:HA	1:B:180:ALA:HB1	2.02	0.41
1:C:273:LEU:HA	1:C:273:LEU:HD12	1.84	0.41
1:D:225:LEU:HD23	1:D:225:LEU:HA	1.69	0.41
1:F:225:LEU:HA	1:F:225:LEU:HD23	1.78	0.41
1:E:387:LEU:HD13	1:E:437:ARG:HG2	2.01	0.41
1:E:432:LEU:O	1:E:437:ARG:NH1	2.54	0.41
1:C:93:MET:HA	1:C:99:TYR:CD2	2.56	0.41
1:D:187:GLN:HG2	1:D:190:GLU:HG3	2.02	0.41
1:E:291:ASP:OD1	1:E:292:LEU:N	2.54	0.41
1:E:380:LEU:HD23	1:E:380:LEU:HA	1.86	0.41
1:E:393:VAL:HG13	1:E:410:LEU:CD2	2.50	0.41
1:A:448:VAL:O	1:A:451:ILE:HG13	2.20	0.41
1:C:307:ILE:HG12	1:C:316:ILE:HD12	2.02	0.41
1:C:472:LEU:HD23	1:C:472:LEU:HA	1.93	0.41
1:E:225:LEU:HD11	1:E:244:ARG:HD3	2.03	0.41
1:A:346:THR:O	1:A:347:LEU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLN:OE1	1:C:158:VAL:HG12	2.20	0.41
1:C:191:ILE:HD13	1:C:191:ILE:HA	1.77	0.41
1:D:168:LEU:HD23	1:D:168:LEU:HA	1.79	0.41
1:D:246:LYS:HE2	1:D:248:GLU:OE2	2.20	0.41
1:E:316:ILE:H	1:E:316:ILE:HG13	1.71	0.41
1:E:387:LEU:HD21	1:E:427:MET:HE1	2.02	0.41
1:E:454:LEU:HD23	1:E:454:LEU:HA	1.84	0.41
1:A:73:GLU:O	1:A:77:LYS:HB2	2.21	0.41
1:B:200:GLU:HG3	1:B:469:ARG:HH21	1.85	0.41
1:B:338:VAL:HB	1:B:343:LYS:HD3	2.03	0.41
1:B:445:GLN:O	1:B:448:VAL:HB	2.22	0.41
1:C:158:VAL:HG23	1:C:159:VAL:HG22	2.03	0.41
1:C:180:ALA:O	1:C:333:ASN:ND2	2.54	0.41
1:D:312:ASN:HB2	1:D:315:VAL:HG23	2.02	0.41
1:E:429:LEU:HA	1:E:429:LEU:HD23	1.83	0.41
1:F:163:ARG:NH1	1:F:471:GLU:OE1	2.53	0.41
1:B:69:ARG:NH1	1:B:73:GLU:HB2	2.35	0.40
1:D:191:ILE:HD13	1:D:213:ILE:HD13	2.03	0.40
1:D:288:GLY:HA2	1:D:308:ARG:HD2	2.03	0.40
1:D:476:LYS:O	1:D:480:ASN:HB2	2.21	0.40
1:E:149:ASN:CG	1:E:154:GLU:H	2.29	0.40
1:B:64:TYR:CD1	1:B:127:ARG:HG2	2.56	0.40
1:C:54:ASN:ND2	1:C:136:LEU:HD22	2.36	0.40
1:C:135:ILE:HA	1:C:162:SER:HA	2.02	0.40
1:E:67:SER:O	1:E:70:ILE:HG23	2.20	0.40
1:F:131:ILE:O	1:F:131:ILE:HG13	2.21	0.40
1:F:265:PRO:O	1:F:268:VAL:HG13	2.21	0.40
1:B:137:ARG:NH1	1:B:471:GLU:HG2	2.36	0.40
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.87	0.40
1:D:67:SER:O	1:D:70:ILE:HG23	2.21	0.40
1:D:413:GLN:HB3	1:D:414:PHE:CD2	2.57	0.40
1:F:259:ILE:HG13	1:F:307:ILE:HD11	2.02	0.40
1:B:149:ASN:N	1:B:149:ASN:OD1	2.53	0.40
1:B:243:ILE:H	1:B:243:ILE:HG13	1.69	0.40
1:B:365:ARG:O	1:B:368:TYR:HB3	2.21	0.40
1:C:95:GLN:C	1:C:97:PHE:H	2.29	0.40
1:C:187:GLN:CG	1:C:190:GLU:H	2.32	0.40
1:C:398:ARG:CZ	1:D:390:LEU:HD23	2.51	0.40
1:A:39:ARG:HD2	1:A:357:HIS:ND1	2.36	0.40
1:A:215:GLY:HA3	1:A:230:ILE:HD13	2.03	0.40
1:A:226:GLY:O	1:A:230:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ASP:HB3	1:D:285:LYS:HE2	2.03	0.40
1:E:78:TYR:HD1	1:E:156:GLU:HB3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	456/502 (91%)	427 (94%)	28 (6%)	1 (0%)	43	71
1	B	455/502 (91%)	422 (93%)	28 (6%)	5 (1%)	11	39
1	C	451/502 (90%)	416 (92%)	35 (8%)	0	100	100
1	D	451/502 (90%)	419 (93%)	31 (7%)	1 (0%)	43	71
1	E	452/502 (90%)	422 (93%)	28 (6%)	2 (0%)	30	60
1	F	448/502 (89%)	426 (95%)	20 (4%)	2 (0%)	30	60
All	All	2713/3012 (90%)	2532 (93%)	170 (6%)	11 (0%)	30	60

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	ALA
1	B	84	SER
1	E	84	SER
1	E	221	ALA
1	B	266	TYR
1	D	221	ALA
1	F	149	ASN
1	A	34	ALA
1	B	34	ALA
1	F	60	SER
1	B	411	ILE

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	393/435 (90%)	350 (89%)	43 (11%)	6	23
1	B	392/435 (90%)	357 (91%)	35 (9%)	9	32
1	C	391/435 (90%)	338 (86%)	53 (14%)	3	16
1	D	392/435 (90%)	342 (87%)	50 (13%)	4	18
1	E	391/435 (90%)	345 (88%)	46 (12%)	5	20
1	F	389/435 (89%)	347 (89%)	42 (11%)	6	23
All	All	2348/2610 (90%)	2079 (88%)	269 (12%)	5	21

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	38	VAL
1	A	45	VAL
1	A	61	ASP
1	A	66	LYS
1	A	75	ILE
1	A	89	SER
1	A	98	ASN
1	A	102	MET
1	A	113	VAL
1	A	117	SER
1	A	130	LYS
1	A	136	LEU
1	A	139	ILE
1	A	140	THR
1	A	143	THR
1	A	159	VAL
1	A	175	ILE
1	A	177	VAL
1	A	179	MET
1	A	181	THR
1	A	195	VAL

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Mol	Chain	Res	Type
1	A	209	LEU
1	A	228	SER
1	A	240	SER
1	A	241	ILE
1	A	256	LYS
1	A	261	VAL
1	A	268	VAL
1	A	280	LEU
1	A	286	ILE
1	A	346	THR
1	A	359	LYS
1	A	398	ARG
1	A	402	THR
1	A	417	THR
1	A	429	LEU
1	A	435	LEU
1	A	445	GLN
1	A	446	SER
1	A	453	GLU
1	A	485	THR
1	A	489	THR
1	B	45	VAL
1	B	50	LEU
1	B	60	SER
1	B	70	ILE
1	B	83	ASP
1	B	84	SER
1	B	98	ASN
1	B	102	MET
1	B	131	ILE
1	B	136	LEU
1	B	140	THR
1	B	182	ASN
1	B	187	GLN
1	B	188	LEU
1	B	203	ASP
1	B	220	THR
1	B	243	ILE
1	B	248	GLU
1	B	252	THR
1	B	258	ARG
1	B	260	ILE

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Mol	Chain	Res	Type
1	B	261	VAL
1	B	274	ILE
1	B	293	ARG
1	B	323	GLN
1	B	326	LEU
1	B	328	THR
1	B	332	ILE
1	B	385	VAL
1	B	395	SER
1	B	413	GLN
1	B	417	THR
1	B	447	LEU
1	B	453	GLU
1	B	458	LEU
1	C	53	MET
1	C	66	LYS
1	C	70	ILE
1	C	75	ILE
1	C	83	ASP
1	C	90	MET
1	C	98	ASN
1	C	102	MET
1	C	131	ILE
1	C	135	ILE
1	C	136	LEU
1	C	140	THR
1	C	144	ILE
1	C	147	GLN
1	C	159	VAL
1	C	162	SER
1	C	175	ILE
1	C	181	THR
1	C	182	ASN
1	C	204	ILE
1	C	210	MET
1	C	240	SER
1	C	241	ILE
1	C	256	LYS
1	C	258	ARG
1	C	262	THR
1	C	268	VAL
1	C	269	ASN

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Mol	Chain	Res	Type
1	C	277	ILE
1	C	280	LEU
1	C	287	GLU
1	C	305	ILE
1	C	308	ARG
1	C	309	ARG
1	C	310	ASP
1	C	323	GLN
1	C	335	LEU
1	C	346	THR
1	C	347	LEU
1	C	398	ARG
1	C	401	GLN
1	C	402	THR
1	C	404	GLU
1	C	413	GLN
1	C	416	LEU
1	C	417	THR
1	C	418	GLU
1	C	432	LEU
1	C	435	LEU
1	C	447	LEU
1	C	453	GLU
1	C	468	ILE
1	C	489	THR
1	D	35	LEU
1	D	45	VAL
1	D	70	ILE
1	D	84	SER
1	D	90	MET
1	D	98	ASN
1	D	102	MET
1	D	112	SER
1	D	131	ILE
1	D	132	SER
1	D	136	LEU
1	D	137	ARG
1	D	140	THR
1	D	144	ILE
1	D	158	VAL
1	D	159	VAL
1	D	169	VAL

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Mol	Chain	Res	Type
1	D	187	GLN
1	D	227	ARG
1	D	236	SER
1	D	241	ILE
1	D	256	LYS
1	D	261	VAL
1	D	262	THR
1	D	263	GLU
1	D	280	LEU
1	D	287	GLU
1	D	305	ILE
1	D	308	ARG
1	D	314	ASN
1	D	323	GLN
1	D	327	GLN
1	D	337	LEU
1	D	347	LEU
1	D	391	ASP
1	D	395	SER
1	D	401	GLN
1	D	402	THR
1	D	413	GLN
1	D	416	LEU
1	D	417	THR
1	D	432	LEU
1	D	445	GLN
1	D	447	LEU
1	D	448	VAL
1	D	453	GLU
1	D	456	ASP
1	D	458	LEU
1	D	484	ARG
1	D	489	THR
1	E	59	THR
1	E	61	ASP
1	E	66	LYS
1	E	70	ILE
1	E	71	VAL
1	E	90	MET
1	E	96	ASP
1	E	98	ASN
1	E	102	MET

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Mol	Chain	Res	Type
1	E	112	SER
1	E	131	ILE
1	E	136	LEU
1	E	137	ARG
1	E	139	ILE
1	E	153	SER
1	E	155	ARG
1	E	158	VAL
1	E	159	VAL
1	E	179	MET
1	E	187	GLN
1	E	227	ARG
1	E	240	SER
1	E	241	ILE
1	E	242	THR
1	E	263	GLU
1	E	268	VAL
1	E	280	LEU
1	E	287	GLU
1	E	308	ARG
1	E	323	GLN
1	E	328	THR
1	E	341	GLN
1	E	347	LEU
1	E	363	ARG
1	E	372	LYS
1	E	391	ASP
1	E	398	ARG
1	E	402	THR
1	E	413	GLN
1	E	435	LEU
1	E	445	GLN
1	E	446	SER
1	E	447	LEU
1	E	453	GLU
1	E	485	THR
1	E	489	THR
1	F	45	VAL
1	F	53	MET
1	F	70	ILE
1	F	75	ILE
1	F	83	ASP

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Mol	Chain	Res	Type
1	F	90	MET
1	F	91	VAL
1	F	98	ASN
1	F	102	MET
1	F	112	SER
1	F	131	ILE
1	F	136	LEU
1	F	137	ARG
1	F	140	THR
1	F	159	VAL
1	F	169	VAL
1	F	179	MET
1	F	203	ASP
1	F	220	THR
1	F	240	SER
1	F	241	ILE
1	F	243	ILE
1	F	251	GLN
1	F	256	LYS
1	F	268	VAL
1	F	280	LEU
1	F	287	GLU
1	F	305	ILE
1	F	308	ARG
1	F	310	ASP
1	F	347	LEU
1	F	398	ARG
1	F	402	THR
1	F	417	THR
1	F	418	GLU
1	F	435	LEU
1	F	440	ILE
1	F	445	GLN
1	F	446	SER
1	F	453	GLU
1	F	457	ILE
1	F	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	107	HIS
1	A	109	ASN
1	A	353	HIS
1	A	422	GLN
1	B	109	ASN
1	B	319	ASN
1	C	81	HIS
1	C	187	GLN
1	C	251	GLN
1	C	269	ASN
1	C	327	GLN
1	C	480	ASN
1	D	107	HIS
1	D	251	GLN
1	D	269	ASN
1	D	353	HIS
1	D	357	HIS
1	D	480	ASN
1	E	79	HIS
1	E	81	HIS
1	E	107	HIS
1	E	187	GLN
1	E	312	ASN
1	E	314	ASN
1	E	349	GLN
1	E	389	HIS
1	F	79	HIS
1	F	81	HIS
1	F	269	ASN
1	F	389	HIS

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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TRS	F	602	-	7,7,7	0.29	0	9,9,9	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	F	602	-	-	5/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	602	TRS	C1-C-C3-O3
3	F	602	TRS	N-C-C3-O3
3	F	602	TRS	C2-C-C3-O3
3	F	602	TRS	C3-C-C2-O2
3	F	602	TRS	N-C-C2-O2

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	458/502 (91%)	-0.71	0	100	100	94, 136, 222, 293	0
1	B	457/502 (91%)	-0.80	0	100	100	97, 127, 162, 231	0
1	C	455/502 (90%)	-0.76	1 (0%)	91	86	92, 129, 176, 232	0
1	D	455/502 (90%)	-0.78	1 (0%)	91	86	101, 139, 211, 287	0
1	E	456/502 (90%)	-0.73	0	100	100	93, 142, 231, 287	0
1	F	452/502 (90%)	-0.67	1 (0%)	91	86	110, 152, 196, 247	0
All	All	2733/3012 (90%)	-0.74	3 (0%)	92	90	92, 137, 205, 293	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	175	ILE	3.2
1	F	180	ALA	2.3
1	C	34	ALA	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 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	K	B	601	1/1	0.60	0.10	210,210,210,210	0
2	K	E	601	1/1	0.77	0.04	195,195,195,195	0
2	K	F	601	1/1	0.84	0.06	179,179,179,179	0
2	K	C	601	1/1	0.85	0.08	180,180,180,180	0
2	K	A	601	1/1	0.88	0.06	181,181,181,181	0
3	TRS	F	602	8/8	0.90	0.10	138,165,167,169	0
2	K	D	601	1/1	0.94	0.05	166,166,166,166	0

6.5 Other polymers [i](#)

There are no such residues in this entry.