



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:49 PM UTC

PDB ID : 3IG1 / pdb_00003ig1
Title : HIV-1 Reverse Transcriptase with the Inhibitor beta-Thujaplicinol Bound at the RNase H Active Site
Authors : Himmel, D.M.; Maegley, K.A.; Pauly, T.A.; Arnold, E.
Deposited on : 2009-07-27
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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

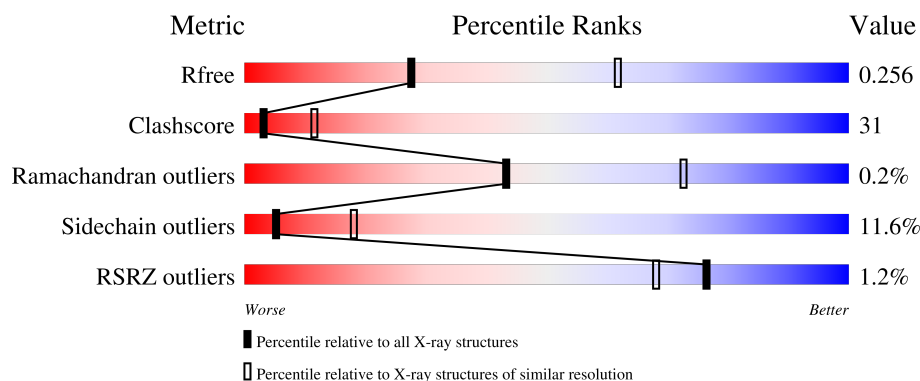
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	555	
2	B	428	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7964 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 HIV-1 Reverse Transcriptase p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4489	2902	748	832	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	SER	PHE	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

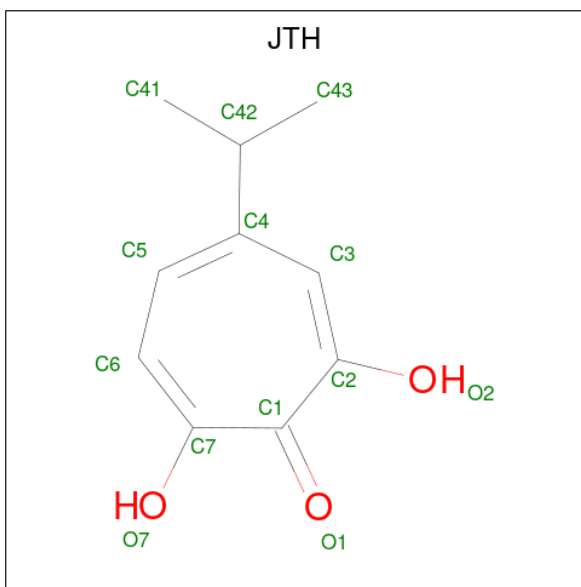
- Molecule 2 is a protein called HIV-1 Reverse Transcriptase p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	409	Total	C	N	O	S	0	0	0
			3386	2208	560	611	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 2,7-dihydroxy-4-(propan-2-yl)cyclohepta-2,4,6-trien-1-one (CCD ID: JTH) (formula: C₁₀H₁₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	10	3		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

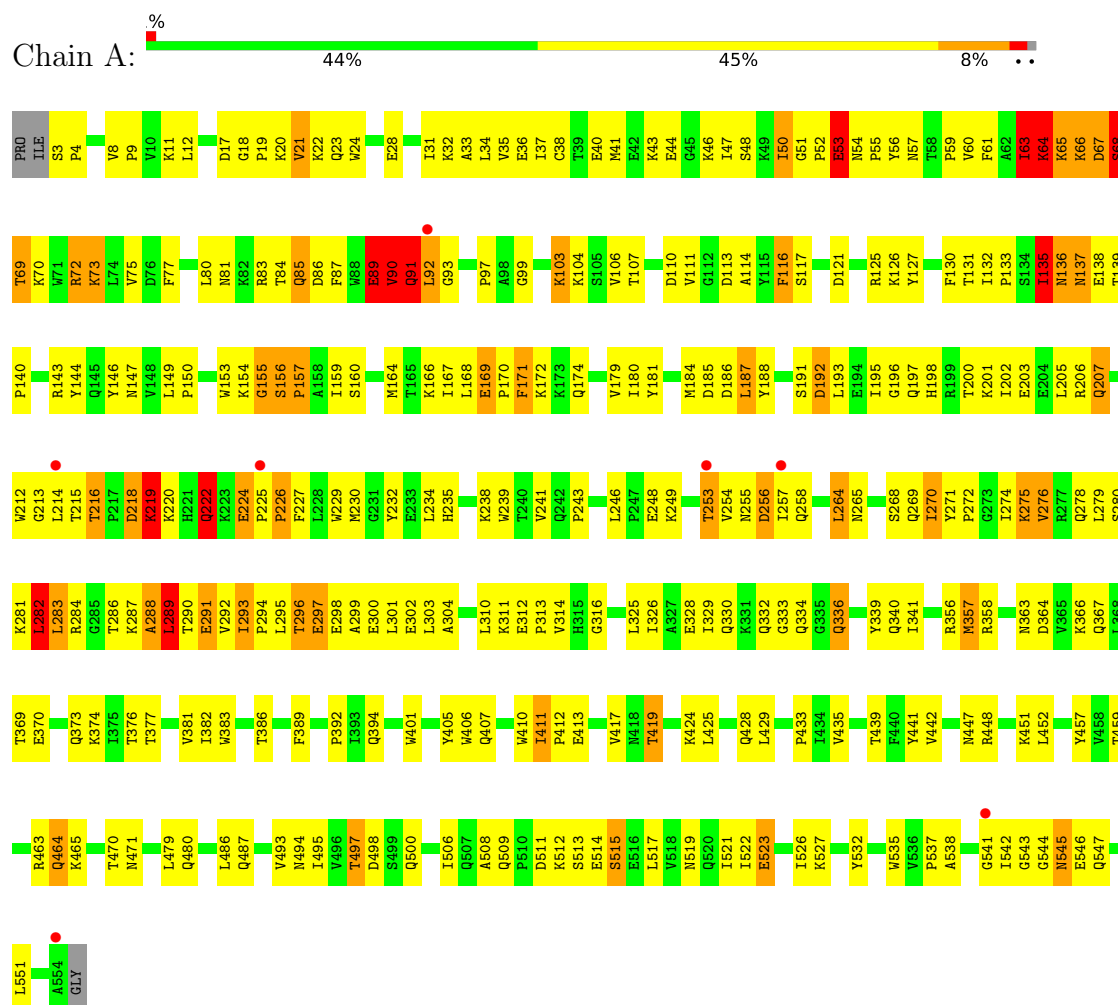
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total	O	0	0
			46	46		
5	B	28	Total	O	0	0
			28	28		

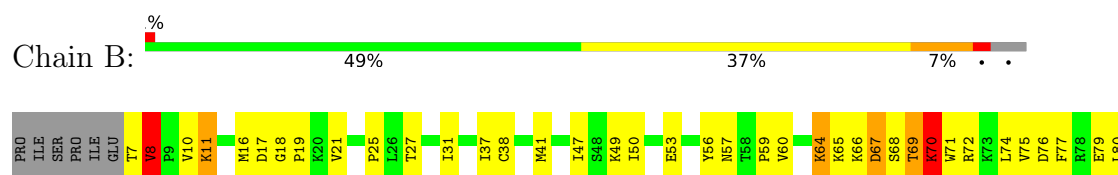
3 Residue-property plots

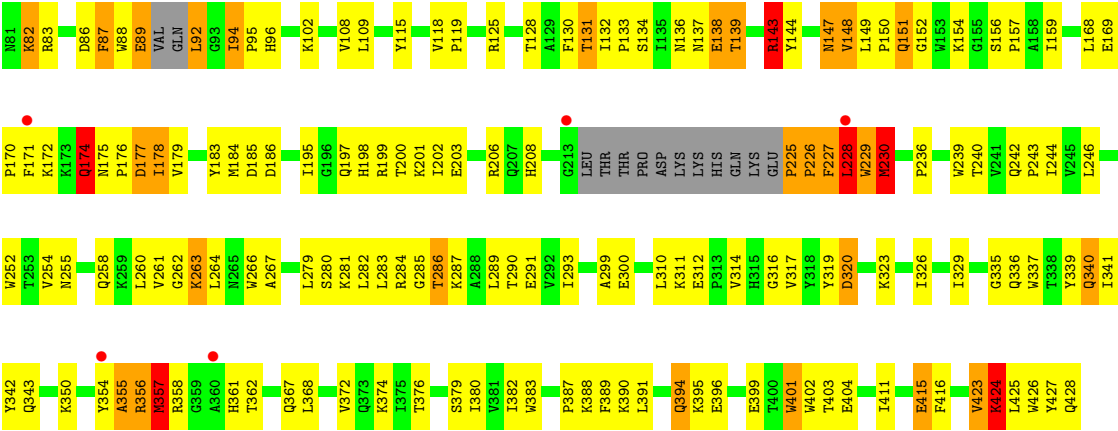
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HIV-1 Reverse Transcriptase p66 subunit



• Molecule 2: HIV-1 Reverse Transcriptase p51 subunit





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.06Å 71.30Å 108.54Å 90.00° 105.13° 90.00°	Depositor
Resolution (Å)	33.75 – 2.80 33.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.9 (33.75-2.80) 91.8 (33.75-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.255 0.236 , 0.256	Depositor DCC
R_{free} test set	801 reflections (2.79%)	wwPDB-VP
Wilson B-factor (Å ²)	66.4	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7964	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: JTH, MN

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	0.61	5/4605 (0.1%)	1.32	77/6256 (1.2%)
2	B	0.49	3/3485 (0.1%)	1.25	50/4732 (1.1%)
All	All	0.56	8/8090 (0.1%)	1.29	127/10988 (1.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	LYS	N-CA	7.15	1.55	1.46
1	A	90	VAL	N-CA	6.70	1.54	1.46
1	A	91	GLN	CA-C	-5.72	1.46	1.53
2	B	227	PHE	CA-C	-5.40	1.46	1.52
2	B	228	LEU	N-CA	-5.28	1.40	1.46
1	A	192	ASP	N-CA	-5.19	1.39	1.46
1	A	91	GLN	N-CA	-5.04	1.40	1.46
2	B	357	MET	N-CA	-5.03	1.39	1.45

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	VAL	N-CA-C	16.73	123.02	108.63
1	A	293	ILE	N-CA-C	16.40	125.77	107.89
2	B	357	MET	N-CA-C	-15.45	88.19	110.59
2	B	226	PRO	CA-C-N	-13.76	101.55	122.74
2	B	226	PRO	C-N-CA	-13.76	101.55	122.74
1	A	545	ASN	N-CA-C	-12.36	97.98	113.55
1	A	53	GLU	N-CA-C	11.84	127.21	113.01
1	A	288	ALA	N-CA-C	11.53	127.69	108.90
1	A	294	PRO	CB-CA-C	11.37	126.88	110.63
1	A	197	GLN	N-CA-C	-10.47	101.00	113.88
2	B	174	GLN	OE1-CD-NE2	-10.45	112.15	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	151	GLN	OE1-CD-NE2	-10.37	112.23	122.60
1	A	207	GLN	OE1-CD-NE2	-10.37	112.23	122.60
2	B	70	LYS	N-CA-C	10.19	126.00	109.59
1	A	222	GLN	OE1-CD-NE2	-10.18	112.42	122.60
1	A	85	GLN	OE1-CD-NE2	-10.17	112.43	122.60
1	A	91	GLN	OE1-CD-NE2	-10.07	112.53	122.60
1	A	135	ILE	N-CA-C	9.96	119.99	110.42
1	A	283	LEU	N-CA-C	9.37	125.51	107.71
1	A	226	PRO	CB-CA-C	9.35	126.99	111.56
1	A	464	GLN	OE1-CD-NE2	-9.21	113.39	122.60
2	B	356	ARG	N-CA-C	9.19	120.83	107.88
1	A	219	LYS	N-CA-C	8.95	123.72	110.48
1	A	293	ILE	N-CA-CB	-8.73	102.27	111.61
1	A	218	ASP	N-CA-C	-8.69	97.44	109.95
2	B	177	ASP	N-CA-C	8.57	123.79	113.16
1	A	287	LYS	CA-C-N	-8.55	110.94	122.99
1	A	287	LYS	C-N-CA	-8.55	110.94	122.99
1	A	103	LYS	N-CA-C	-8.54	96.75	109.81
1	A	69	THR	N-CA-C	8.45	122.69	110.10
1	A	289	LEU	N-CA-C	-8.40	99.94	112.04
2	B	357	MET	CA-C-N	-8.18	109.94	122.05
2	B	357	MET	C-N-CA	-8.18	109.94	122.05
1	A	296	THR	N-CA-C	8.04	122.40	112.59
1	A	287	LYS	N-CA-C	8.03	122.78	109.46
1	A	224	GLU	N-CA-C	7.94	127.37	109.81
1	A	89	GLU	N-CA-C	-7.93	98.28	110.10
1	A	493	VAL	N-CA-C	7.84	118.09	108.06
2	B	87	PHE	N-CA-C	7.72	122.50	107.98
1	A	256	ASP	N-CA-C	-7.68	104.40	114.31
1	A	298	GLU	N-CA-C	-7.68	101.06	113.19
2	B	228	LEU	CB-CA-C	-7.61	99.26	111.28
2	B	391	LEU	N-CA-C	7.56	119.17	109.72
1	A	224	GLU	CA-C-N	7.56	128.16	120.38
1	A	224	GLU	C-N-CA	7.56	128.16	120.38
2	B	382	ILE	N-CA-C	7.54	119.22	111.00
2	B	316	GLY	N-CA-C	7.53	127.10	115.72
2	B	230	MET	N-CA-C	7.50	121.38	110.28
2	B	320	ASP	CA-C-N	7.48	128.15	119.47
2	B	320	ASP	C-N-CA	7.48	128.15	119.47
1	A	300	GLU	N-CA-C	-7.27	104.22	113.23
2	B	174	GLN	CG-CD-NE2	7.14	127.11	116.40
1	A	91	GLN	CG-CD-NE2	7.07	127.01	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	LYS	N-CA-C	7.06	119.48	108.96
2	B	151	GLN	CG-CD-NE2	7.03	126.94	116.40
1	A	207	GLN	CG-CD-NE2	6.97	126.85	116.40
2	B	362	THR	N-CA-C	6.90	121.36	113.15
1	A	222	GLN	CG-CD-NE2	6.88	126.72	116.40
1	A	140	PRO	CB-CA-C	6.86	120.34	111.21
1	A	282	LEU	N-CA-C	-6.77	104.84	113.23
1	A	155	GLY	N-CA-C	6.75	124.16	115.32
1	A	64	LYS	N-CA-C	6.69	119.20	110.43
1	A	85	GLN	CG-CD-NE2	6.67	126.40	116.40
1	A	464	GLN	CG-CD-NE2	6.64	126.36	116.40
2	B	355	ALA	CA-C-N	-6.63	110.64	122.45
2	B	355	ALA	C-N-CA	-6.63	110.64	122.45
1	A	508	ALA	N-CA-C	-6.55	105.33	113.38
1	A	479	LEU	N-CA-C	-6.41	104.37	111.36
2	B	200	THR	N-CA-C	-6.40	103.81	111.69
1	A	191	SER	CA-C-N	-6.37	113.99	122.85
1	A	191	SER	C-N-CA	-6.37	113.99	122.85
1	A	216	THR	CA-C-N	-6.36	111.66	120.25
1	A	216	THR	C-N-CA	-6.36	111.66	120.25
1	A	270	ILE	N-CA-C	-6.34	106.10	111.56
1	A	67	ASP	N-CA-C	-6.34	105.51	113.18
2	B	227	PHE	O-C-N	6.32	130.71	123.31
2	B	312	GLU	N-CA-C	-6.20	102.05	110.36
1	A	91	GLN	N-CA-C	-6.14	95.59	107.44
1	A	114	ALA	N-CA-C	6.11	120.35	113.01
2	B	143	ARG	N-CA-C	6.11	118.91	109.07
1	A	358	ARG	N-CA-C	6.08	119.19	110.24
2	B	227	PHE	CA-CB-CG	-6.08	107.72	113.80
2	B	317	VAL	N-CA-C	6.05	121.92	109.34
2	B	424	LYS	N-CA-C	-5.99	104.87	111.82
2	B	94	ILE	N-CA-C	5.97	121.77	108.88
2	B	18	GLY	CA-C-N	5.96	127.56	120.23
2	B	18	GLY	C-N-CA	5.96	127.56	120.23
2	B	64	LYS	N-CA-C	-5.96	100.00	109.59
1	A	389	PHE	N-CA-C	5.92	118.59	109.07
1	A	68	SER	N-CA-C	-5.88	98.29	108.52
2	B	96	HIS	CA-C-N	5.87	127.18	119.84
2	B	96	HIS	C-N-CA	5.87	127.18	119.84
1	A	90	VAL	N-CA-C	5.83	121.47	109.34
1	A	63	ILE	N-CA-C	5.78	115.58	108.53
2	B	225	PRO	CA-C-N	5.76	126.51	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	225	PRO	C-N-CA	5.76	126.51	120.12
1	A	287	LYS	O-C-N	-5.75	116.67	123.22
2	B	147	ASN	N-CA-C	-5.73	104.86	112.94
2	B	358	ARG	N-CA-C	5.71	118.18	109.62
1	A	514	GLU	N-CA-C	-5.69	106.55	112.93
2	B	401	TRP	N-CA-CB	-5.69	103.47	110.98
1	A	12	LEU	N-CA-C	-5.68	103.03	110.53
2	B	69	THR	CB-CA-C	-5.65	98.17	109.99
1	A	364	ASP	N-CA-C	5.63	118.14	111.33
1	A	401	TRP	N-CA-C	5.58	117.23	111.03
1	A	283	LEU	CB-CA-C	-5.58	103.56	111.76
1	A	52	PRO	CA-C-N	5.55	132.17	121.18
1	A	52	PRO	C-N-CA	5.55	132.17	121.18
2	B	227	PHE	CA-C-O	5.54	126.47	120.32
2	B	343	GLN	N-CA-C	-5.52	107.20	114.04
1	A	184	MET	CB-CA-C	-5.48	108.67	116.34
1	A	294	PRO	N-CA-C	-5.46	102.56	111.68
1	A	90	VAL	CB-CA-C	-5.46	102.34	111.29
2	B	227	PHE	CA-C-N	5.45	131.67	122.79
2	B	227	PHE	C-N-CA	5.45	131.67	122.79
1	A	224	GLU	O-C-N	5.42	127.55	121.32
2	B	19	PRO	N-CA-C	5.40	118.97	110.50
2	B	184	MET	CB-CA-C	-5.39	110.34	116.54
2	B	227	PHE	N-CA-C	5.32	117.75	108.76
1	A	222	GLN	N-CA-C	5.32	118.15	107.41
1	A	91	GLN	CA-C-N	-5.27	114.12	122.23
1	A	91	GLN	C-N-CA	-5.27	114.12	122.23
1	A	275	LYS	N-CA-C	5.25	116.70	109.15
1	A	171	PHE	N-CA-C	-5.22	105.65	112.23
1	A	303	LEU	N-CA-C	-5.10	105.71	112.34
1	A	286	THR	CA-C-N	5.09	129.37	122.19
1	A	286	THR	C-N-CA	5.09	129.37	122.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4489	0	4545	329	0
2	B	3386	0	3412	189	0
3	A	13	0	10	0	0
4	A	2	0	0	0	0
5	A	46	0	0	2	0
5	B	28	0	0	1	0
All	All	7964	0	7967	495	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 31.

All (495) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:CB	1:A:225:PRO:HD2	1.48	1.35
2:B:227:PHE:HB3	2:B:229:TRP:CD1	1.64	1.33
2:B:226:PRO:O	2:B:227:PHE:CD1	1.89	1.26
1:A:224:GLU:HB2	1:A:225:PRO:CD	1.62	1.25
1:A:224:GLU:C	1:A:226:PRO:HD2	1.68	1.19
1:A:72:ARG:HB2	1:A:72:ARG:NH1	1.59	1.16
1:A:28:GLU:HG2	1:A:135:ILE:CG1	1.76	1.15
1:A:224:GLU:CB	1:A:225:PRO:CD	2.20	1.14
2:B:225:PRO:HB2	2:B:226:PRO:CD	1.79	1.13
2:B:92:LEU:N	2:B:92:LEU:HD23	1.63	1.13
1:A:28:GLU:HG2	1:A:135:ILE:HG13	1.24	1.13
2:B:225:PRO:CB	2:B:226:PRO:CD	2.26	1.12
1:A:63:ILE:HG13	1:A:64:LYS:HD2	1.18	1.12
1:A:136:ASN:HD21	1:A:138:GLU:CG	1.65	1.09
1:A:136:ASN:HD21	1:A:138:GLU:HG2	1.13	1.07
1:A:64:LYS:HD3	1:A:64:LYS:O	1.53	1.06
2:B:225:PRO:HB3	2:B:226:PRO:HD3	1.37	1.05
2:B:225:PRO:HB2	2:B:226:PRO:HD2	1.33	1.04
2:B:225:PRO:CB	2:B:226:PRO:HD3	1.85	1.03
1:A:72:ARG:HH11	1:A:72:ARG:CB	1.72	1.01
1:A:21:VAL:HG11	1:A:59:PRO:HG3	1.41	1.00
2:B:227:PHE:HB3	2:B:229:TRP:HD1	1.17	0.99
1:A:229:TRP:O	1:A:230:MET:HG3	1.63	0.98
2:B:228:LEU:CG	2:B:228:LEU:O	2.11	0.97
1:A:220:LYS:O	1:A:220:LYS:HG2	1.65	0.94
1:A:72:ARG:HB2	1:A:72:ARG:HH11	0.79	0.93
1:A:28:GLU:CG	1:A:135:ILE:HG13	1.99	0.92
1:A:180:ILE:HG23	1:A:187:LEU:HD11	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LYS:NZ	2:B:227:PHE:CD2	2.40	0.90
2:B:227:PHE:CB	2:B:229:TRP:CD1	2.54	0.89
1:A:290:THR:O	1:A:290:THR:HG22	1.72	0.88
2:B:395:LYS:O	2:B:399:GLU:HG3	1.73	0.88
2:B:228:LEU:O	2:B:228:LEU:HG	1.63	0.87
1:A:21:VAL:HG11	1:A:59:PRO:CG	2.05	0.87
2:B:92:LEU:N	2:B:92:LEU:CD2	2.38	0.87
1:A:276:VAL:HG23	1:A:276:VAL:O	1.75	0.86
1:A:283:LEU:O	1:A:283:LEU:HG	1.75	0.86
1:A:136:ASN:ND2	1:A:138:GLU:HG2	1.91	0.85
2:B:356:ARG:HB2	2:B:357:MET:O	1.76	0.85
1:A:172:LYS:HE2	1:A:180:ILE:HB	1.59	0.85
1:A:224:GLU:HB2	1:A:225:PRO:HD2	0.84	0.84
1:A:225:PRO:N	1:A:226:PRO:CD	2.41	0.83
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.60	0.83
2:B:57:ASN:OD1	2:B:131:THR:HG23	1.79	0.83
1:A:65:LYS:NZ	1:A:65:LYS:HA	1.94	0.83
1:A:544:GLY:HA3	2:B:286:THR:HG23	1.60	0.82
2:B:41:MET:HE3	2:B:47:ILE:HD13	1.62	0.82
1:A:253:THR:HG23	1:A:256:ASP:HB2	1.62	0.82
2:B:8:VAL:HG11	2:B:159:ILE:HG23	1.61	0.82
1:A:167:ILE:O	1:A:170:PRO:HD2	1.80	0.81
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.59	0.81
1:A:229:TRP:O	1:A:230:MET:CG	2.29	0.80
1:A:185:ASP:OD1	1:A:186:ASP:CG	2.25	0.80
1:A:225:PRO:N	1:A:226:PRO:HD2	1.95	0.80
2:B:226:PRO:O	2:B:227:PHE:HD1	1.63	0.80
1:A:216:THR:HG23	1:A:216:THR:O	1.81	0.80
2:B:354:TYR:CE2	2:B:374:LYS:HD3	2.18	0.79
1:A:28:GLU:HG2	1:A:135:ILE:HG12	1.65	0.78
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.19	0.78
2:B:228:LEU:O	2:B:228:LEU:CD1	2.31	0.78
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.19	0.77
1:A:257:ILE:HG22	1:A:283:LEU:HD22	1.66	0.77
1:A:64:LYS:HD3	1:A:64:LYS:C	2.04	0.76
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.14	0.76
2:B:228:LEU:O	2:B:228:LEU:HD12	1.86	0.76
1:A:32:LYS:O	1:A:35:VAL:HG12	1.86	0.76
2:B:254:VAL:HG22	2:B:293:ILE:HD11	1.66	0.75
1:A:28:GLU:CG	1:A:135:ILE:CG1	2.61	0.75
2:B:356:ARG:CB	2:B:357:MET:O	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLY:H	1:A:547:GLN:HG2	1.51	0.74
1:A:21:VAL:CG1	1:A:59:PRO:HG3	2.16	0.74
1:A:136:ASN:ND2	1:A:138:GLU:CG	2.48	0.74
1:A:169:GLU:O	1:A:169:GLU:HG3	1.87	0.73
1:A:181:TYR:CD2	2:B:138:GLU:HG3	2.23	0.73
2:B:229:TRP:CE3	2:B:230:MET:HG2	2.24	0.73
1:A:301:LEU:O	1:A:304:ALA:HB3	1.89	0.72
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.33	0.72
2:B:227:PHE:HB3	2:B:229:TRP:NE1	2.04	0.72
1:A:138:GLU:HG3	1:A:139:THR:HG23	1.72	0.72
1:A:65:LYS:HG2	1:A:72:ARG:CZ	2.20	0.72
1:A:90:VAL:HG13	1:A:91:GLN:H	1.55	0.71
1:A:65:LYS:HA	1:A:65:LYS:HZ3	1.57	0.70
1:A:224:GLU:C	1:A:226:PRO:CD	2.56	0.70
2:B:115:TYR:O	2:B:149:LEU:HB2	1.92	0.70
1:A:85:GLN:O	1:A:87:PHE:CE1	2.43	0.70
1:A:181:TYR:CE2	2:B:138:GLU:HG3	2.27	0.70
1:A:136:ASN:ND2	1:A:138:GLU:HB3	2.08	0.69
1:A:254:VAL:HG22	1:A:293:ILE:HD12	1.73	0.69
1:A:254:VAL:HG13	1:A:283:LEU:CD1	2.23	0.69
1:A:441:TYR:HB3	1:A:544:GLY:O	1.93	0.68
1:A:33:ALA:O	1:A:36:GLU:HB2	1.92	0.68
1:A:185:ASP:OD1	1:A:186:ASP:N	2.24	0.68
1:A:291:GLU:HA	1:A:291:GLU:OE1	1.92	0.68
1:A:32:LYS:O	1:A:35:VAL:CG1	2.41	0.68
2:B:134:SER:HB2	2:B:139:THR:HG23	1.74	0.68
2:B:226:PRO:O	2:B:227:PHE:CG	2.44	0.68
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.27	0.67
1:A:149:LEU:HD13	1:A:156:SER:HA	1.76	0.67
1:A:213:GLY:C	1:A:214:LEU:HD12	2.19	0.67
2:B:134:SER:CB	2:B:139:THR:HG23	2.23	0.67
1:A:224:GLU:HB2	1:A:226:PRO:HD3	1.76	0.67
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.76	0.67
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.29	0.67
1:A:180:ILE:CG2	1:A:187:LEU:HD11	2.24	0.67
1:A:99:GLY:HA3	2:B:136:ASN:ND2	2.09	0.67
1:A:111:VAL:HG11	1:A:164:MET:HE1	1.77	0.67
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.77	0.67
1:A:136:ASN:C	1:A:136:ASN:HD22	2.01	0.66
2:B:263:LYS:HB2	2:B:426:TRP:CD1	2.31	0.66
1:A:3:SER:N	1:A:4:PRO:HD2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:ND2	1:A:138:GLU:CB	2.58	0.66
1:A:224:GLU:HB2	1:A:226:PRO:CD	2.25	0.66
2:B:118:VAL:HB	2:B:149:LEU:HG	1.76	0.66
1:A:104:LYS:N	1:A:192:ASP:OD1	2.29	0.65
1:A:136:ASN:HD21	1:A:138:GLU:CB	2.09	0.65
1:A:180:ILE:C	1:A:181:TYR:CD2	2.74	0.65
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.79	0.65
2:B:354:TYR:CZ	2:B:374:LYS:HD3	2.31	0.65
1:A:265:ASN:O	1:A:268:SER:HB2	1.97	0.65
2:B:70:LYS:NZ	2:B:226:PRO:HG2	2.11	0.65
1:A:180:ILE:C	1:A:181:TYR:HD2	2.04	0.65
1:A:288:ALA:HB2	1:A:291:GLU:HB2	1.78	0.65
1:A:441:TYR:CB	1:A:544:GLY:O	2.44	0.65
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.94	0.65
1:A:511:ASP:O	1:A:512:LYS:HG3	1.96	0.65
2:B:355:ALA:O	2:B:356:ARG:HB3	1.97	0.65
2:B:356:ARG:CG	2:B:357:MET:O	2.45	0.65
2:B:72:ARG:HG2	2:B:72:ARG:HH11	1.62	0.64
2:B:227:PHE:CB	2:B:229:TRP:NE1	2.60	0.64
1:A:203:GLU:O	1:A:207:GLN:HG3	1.96	0.64
1:A:93:GLY:HA3	2:B:137:ASN:ND2	2.13	0.64
1:A:279:LEU:CD2	1:A:299:ALA:HB1	2.28	0.64
1:A:382:ILE:O	2:B:136:ASN:HB2	1.97	0.64
2:B:356:ARG:HG3	2:B:357:MET:O	1.97	0.64
1:A:279:LEU:HD21	1:A:299:ALA:HB1	1.79	0.64
2:B:174:GLN:O	2:B:176:PRO:HD3	1.97	0.64
1:A:93:GLY:HA3	2:B:137:ASN:HD21	1.64	0.63
1:A:424:LYS:CG	1:A:425:LEU:H	2.10	0.63
1:A:213:GLY:O	1:A:214:LEU:HD12	1.98	0.63
1:A:216:THR:O	1:A:216:THR:CG2	2.46	0.63
2:B:254:VAL:HG12	2:B:258:GLN:NE2	2.13	0.62
1:A:543:GLY:HA3	2:B:285:GLY:O	1.98	0.62
2:B:148:VAL:O	2:B:150:PRO:HD3	1.99	0.62
2:B:31:ILE:HD13	2:B:133:PRO:O	1.98	0.62
1:A:33:ALA:O	1:A:36:GLU:N	2.33	0.62
2:B:138:GLU:HG2	2:B:139:THR:N	2.13	0.62
2:B:70:LYS:HZ1	2:B:226:PRO:HG2	1.64	0.62
1:A:8:VAL:O	1:A:121:ASP:HB2	2.00	0.61
1:A:21:VAL:CG1	1:A:22:LYS:N	2.63	0.61
2:B:70:LYS:HZ1	2:B:226:PRO:CD	2.14	0.61
2:B:394:GLN:NE2	2:B:396:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:LYS:HG3	2:B:425:LEU:N	2.13	0.61
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.35	0.61
1:A:85:GLN:NE2	2:B:53:GLU:O	2.33	0.61
2:B:8:VAL:HG11	2:B:159:ILE:CG2	2.31	0.61
2:B:361:HIS:HB3	2:B:367:GLN:NE2	2.16	0.60
1:A:254:VAL:HG13	1:A:283:LEU:HD12	1.83	0.60
2:B:229:TRP:CD1	2:B:229:TRP:H	2.17	0.60
1:A:164:MET:HG3	1:A:168:LEU:CD1	2.31	0.60
1:A:257:ILE:HD11	1:A:295:LEU:HD21	1.83	0.60
1:A:333:GLY:O	1:A:336:GLN:HB2	2.01	0.60
2:B:70:LYS:HZ1	2:B:226:PRO:CG	2.14	0.60
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.02	0.60
1:A:185:ASP:OD1	1:A:186:ASP:OD1	2.19	0.59
1:A:84:THR:O	1:A:154:LYS:NZ	2.35	0.59
1:A:31:ILE:HD13	1:A:133:PRO:O	2.02	0.59
1:A:283:LEU:O	1:A:283:LEU:CG	2.47	0.59
1:A:366:LYS:O	1:A:370:GLU:HG3	2.03	0.59
1:A:283:LEU:O	1:A:284:ARG:HG2	2.02	0.59
1:A:11:LYS:O	1:A:85:GLN:HB3	2.02	0.59
2:B:281:LYS:HE2	2:B:284:ARG:NH2	2.18	0.59
1:A:271:TYR:CE2	1:A:314:VAL:HG23	2.38	0.58
2:B:178:ILE:CG2	2:B:179:VAL:N	2.66	0.58
2:B:70:LYS:HZ1	2:B:226:PRO:HD2	1.68	0.58
2:B:319:TYR:CD2	2:B:383:TRP:HD1	2.21	0.58
2:B:337:TRP:O	2:B:354:TYR:N	2.36	0.58
1:A:326:ILE:O	1:A:341:ILE:HA	2.04	0.58
2:B:242:GLN:NE2	2:B:243:PRO:HD2	2.19	0.58
1:A:168:LEU:C	1:A:170:PRO:HD2	2.29	0.58
1:A:137:ASN:OD1	1:A:137:ASN:N	2.36	0.57
1:A:297:GLU:O	1:A:297:GLU:OE2	2.22	0.57
1:A:424:LYS:CG	1:A:425:LEU:N	2.67	0.57
1:A:290:THR:O	1:A:290:THR:CG2	2.45	0.57
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.39	0.57
1:A:97:PRO:HD3	1:A:232:TYR:CZ	2.39	0.57
1:A:167:ILE:O	1:A:170:PRO:CD	2.52	0.57
2:B:49:LYS:NZ	5:B:444:HOH:O	2.37	0.57
1:A:113:ASP:O	1:A:113:ASP:OD2	2.22	0.57
2:B:336:GLN:C	2:B:337:TRP:CD1	2.83	0.57
1:A:180:ILE:O	1:A:181:TYR:HD2	1.87	0.57
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.05	0.57
1:A:186:ASP:OD2	1:A:230:MET:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:HIS:O	2:B:202:ILE:HG12	2.04	0.57
2:B:226:PRO:C	2:B:227:PHE:CD1	2.79	0.57
2:B:337:TRP:CZ3	2:B:368:LEU:HD13	2.40	0.57
2:B:178:ILE:HG22	2:B:179:VAL:N	2.20	0.56
1:A:328:GLU:O	1:A:339:TYR:HA	2.05	0.56
2:B:67:ASP:OD1	2:B:67:ASP:C	2.48	0.56
2:B:357:MET:HG3	2:B:361:HIS:CD2	2.40	0.56
1:A:57:ASN:OD1	1:A:131:THR:OG1	2.22	0.56
1:A:91:GLN:O	1:A:93:GLY:N	2.36	0.56
1:A:72:ARG:NH1	1:A:72:ARG:CB	2.48	0.56
2:B:64:LYS:HE3	2:B:71:TRP:CZ2	2.40	0.56
2:B:339:TYR:OH	2:B:350:LYS:HE3	2.05	0.56
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.41	0.56
1:A:544:GLY:N	1:A:547:GLN:HG2	2.21	0.56
1:A:433:PRO:CG	2:B:255:ASN:OD1	2.53	0.56
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.46	0.55
1:A:185:ASP:OD1	1:A:185:ASP:C	2.48	0.55
2:B:229:TRP:CD2	2:B:230:MET:HG2	2.41	0.55
1:A:65:LYS:C	1:A:66:LYS:HG2	2.31	0.55
1:A:80:LEU:HD12	1:A:80:LEU:O	2.05	0.55
1:A:417:VAL:HG22	1:A:419:THR:HG22	1.88	0.55
1:A:511:ASP:OD1	1:A:511:ASP:C	2.48	0.55
1:A:135:ILE:HD12	1:A:135:ILE:O	2.07	0.55
1:A:169:GLU:N	1:A:170:PRO:CD	2.67	0.55
1:A:33:ALA:O	1:A:36:GLU:CB	2.54	0.55
1:A:167:ILE:C	1:A:170:PRO:HD2	2.31	0.55
1:A:369:THR:O	1:A:373:GLN:HG2	2.05	0.55
1:A:48:SER:O	1:A:144:TYR:HA	2.08	0.55
1:A:373:GLN:OE1	2:B:401:TRP:NE1	2.40	0.55
1:A:457:TYR:CD1	1:A:457:TYR:C	2.85	0.55
1:A:65:LYS:HG2	1:A:72:ARG:NH1	2.22	0.54
1:A:500:GLN:HG2	1:A:535:TRP:HE1	1.73	0.54
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.42	0.54
1:A:135:ILE:O	1:A:135:ILE:CD1	2.56	0.54
2:B:57:ASN:OD1	2:B:131:THR:CG2	2.53	0.54
2:B:226:PRO:C	2:B:227:PHE:CG	2.86	0.54
1:A:136:ASN:C	1:A:137:ASN:CG	2.75	0.54
2:B:388:LYS:HE3	2:B:415:GLU:HG2	1.89	0.54
2:B:7:THR:CG2	2:B:119:PRO:HG2	2.38	0.53
1:A:542:ILE:HG23	2:B:283:LEU:CD1	2.36	0.53
1:A:356:ARG:HG3	1:A:367:GLN:CD	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.44	0.53
2:B:86:ASP:HB3	2:B:88:TRP:CZ2	2.43	0.52
1:A:63:ILE:CG1	1:A:64:LYS:H	2.22	0.52
1:A:274:ILE:O	1:A:274:ILE:HG22	2.08	0.52
1:A:24:TRP:HD1	1:A:61:PHE:HE2	1.57	0.52
1:A:181:TYR:CD2	1:A:181:TYR:N	2.77	0.52
1:A:464:GLN:OE1	1:A:551:LEU:HD11	2.10	0.52
2:B:86:ASP:CB	2:B:88:TRP:CH2	2.93	0.52
2:B:108:VAL:C	2:B:109:LEU:HD12	2.34	0.52
1:A:41:MET:HE3	1:A:116:PHE:CZ	2.45	0.52
1:A:224:GLU:CB	1:A:226:PRO:HD2	2.39	0.52
1:A:332:GLN:HB3	1:A:336:GLN:HB3	1.90	0.52
1:A:448:ARG:O	1:A:451:LYS:NZ	2.34	0.52
1:A:452:LEU:HD22	1:A:470:THR:HG22	1.92	0.52
1:A:164:MET:HG3	1:A:168:LEU:HD11	1.92	0.52
1:A:164:MET:HG3	1:A:168:LEU:HD12	1.92	0.52
2:B:227:PHE:CB	2:B:229:TRP:HD1	2.06	0.52
1:A:523:GLU:OE1	1:A:527:LYS:NZ	2.42	0.52
1:A:136:ASN:C	1:A:137:ASN:OD1	2.53	0.52
1:A:66:LYS:HB2	1:A:68:SER:OG	2.10	0.51
1:A:229:TRP:C	1:A:230:MET:CG	2.82	0.51
2:B:227:PHE:CB	2:B:229:TRP:HE1	2.22	0.51
1:A:21:VAL:HG11	1:A:59:PRO:CD	2.40	0.51
1:A:89:GLU:CB	1:A:92:LEU:HD13	2.40	0.51
1:A:111:VAL:HG11	1:A:164:MET:CE	2.40	0.51
1:A:125:ARG:NH1	1:A:147:ASN:OD1	2.44	0.51
2:B:125:ARG:O	2:B:128:THR:OG1	2.28	0.51
2:B:75:VAL:HG11	2:B:77:PHE:CE1	2.45	0.51
2:B:395:LYS:HA	2:B:416:PHE:CE2	2.46	0.51
2:B:354:TYR:OH	2:B:374:LYS:HB3	2.10	0.51
2:B:79:GLU:OE2	2:B:82:LYS:NZ	2.43	0.51
1:A:410:TRP:O	1:A:411:ILE:HD13	2.10	0.51
1:A:50:ILE:HG13	1:A:143:ARG:CB	2.41	0.51
1:A:166:LYS:O	1:A:170:PRO:HD3	2.11	0.51
1:A:91:GLN:C	1:A:93:GLY:N	2.70	0.50
1:A:50:ILE:CD1	1:A:143:ARG:HB3	2.41	0.50
1:A:90:VAL:HG22	1:A:91:GLN:N	2.21	0.50
1:A:283:LEU:O	1:A:284:ARG:CG	2.59	0.50
1:A:433:PRO:HG3	2:B:255:ASN:OD1	2.10	0.50
1:A:63:ILE:HG13	1:A:64:LYS:H	1.77	0.50
1:A:64:LYS:N	1:A:64:LYS:CD	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASP:HA	1:A:154:LYS:HZ1	1.77	0.50
1:A:271:TYR:HE2	1:A:312:GLU:O	1.94	0.50
2:B:169:GLU:N	2:B:170:PRO:HD2	2.26	0.50
2:B:70:LYS:NZ	2:B:226:PRO:HD2	2.27	0.50
1:A:235:HIS:HB2	1:A:238:LYS:O	2.11	0.49
1:A:275:LYS:O	1:A:302:GLU:CD	2.55	0.49
1:A:412:PRO:HG3	2:B:401:TRP:CH2	2.47	0.49
1:A:64:LYS:HA	1:A:70:LYS:O	2.12	0.49
1:A:222:GLN:CD	1:A:222:GLN:H	2.19	0.49
1:A:271:TYR:CE2	1:A:314:VAL:CG2	2.94	0.49
1:A:255:ASN:ND2	1:A:255:ASN:O	2.45	0.49
1:A:224:GLU:CA	1:A:226:PRO:HD2	2.40	0.49
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.92	0.49
1:A:220:LYS:O	1:A:220:LYS:CG	2.50	0.49
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.06	0.49
1:A:363:ASN:OD1	1:A:363:ASN:C	2.56	0.49
1:A:9:PRO:HA	1:A:121:ASP:OD1	2.13	0.49
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.47	0.49
1:A:254:VAL:HG22	1:A:293:ILE:CD1	2.42	0.49
1:A:497:THR:OG1	1:A:498:ASP:N	2.45	0.49
2:B:287:LYS:HD3	2:B:291:GLU:CD	2.38	0.49
1:A:3:SER:N	1:A:4:PRO:CD	2.75	0.49
1:A:51:GLY:HA3	1:A:53:GLU:OE2	2.13	0.49
1:A:156:SER:N	1:A:157:PRO:CD	2.76	0.49
2:B:88:TRP:O	2:B:89:GLU:HG3	2.12	0.49
2:B:326:ILE:O	2:B:341:ILE:HA	2.13	0.48
1:A:17:ASP:OD2	1:A:18:GLY:N	2.41	0.48
1:A:381:VAL:HG22	2:B:25:PRO:HB3	1.95	0.48
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.95	0.48
1:A:513:SER:O	1:A:519:ASN:ND2	2.32	0.48
2:B:72:ARG:HG2	2:B:72:ARG:NH1	2.28	0.48
1:A:56:TYR:CE2	1:A:127:TYR:CE1	3.02	0.48
2:B:227:PHE:HB2	2:B:229:TRP:HE1	1.77	0.48
1:A:149:LEU:HB3	1:A:156:SER:HB3	1.95	0.48
1:A:441:TYR:CE1	2:B:286:THR:HG22	2.49	0.48
2:B:88:TRP:C	2:B:89:GLU:HG3	2.39	0.48
2:B:195:ILE:HG12	2:B:199:ARG:CD	2.44	0.48
1:A:91:GLN:C	1:A:93:GLY:H	2.22	0.48
1:A:225:PRO:CD	1:A:226:PRO:HD3	2.44	0.48
1:A:283:LEU:C	1:A:284:ARG:HG2	2.37	0.48
2:B:423:VAL:HG23	2:B:423:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.74	0.48
1:A:411:ILE:HG22	1:A:412:PRO:O	2.13	0.48
2:B:7:THR:HG21	2:B:119:PRO:HG2	1.95	0.48
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.49	0.47
1:A:424:LYS:HG2	1:A:425:LEU:N	2.29	0.47
1:A:417:VAL:O	1:A:417:VAL:HG13	2.13	0.47
1:A:541:GLY:HA2	1:A:546:GLU:HG3	1.96	0.47
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.96	0.47
2:B:319:TYR:CD2	2:B:383:TRP:CD1	3.02	0.47
1:A:54:ASN:OD1	1:A:55:PRO:N	2.47	0.47
1:A:85:GLN:O	1:A:87:PHE:CD1	2.66	0.47
1:A:180:ILE:HG23	1:A:187:LEU:CD1	2.35	0.47
2:B:395:LYS:HB2	2:B:416:PHE:CD1	2.50	0.47
1:A:65:LYS:O	1:A:66:LYS:HG2	2.14	0.47
1:A:243:PRO:CG	1:A:313:PRO:HG3	2.45	0.47
2:B:357:MET:CB	2:B:361:HIS:HD2	2.27	0.47
2:B:401:TRP:O	2:B:404:GLU:HB2	2.14	0.47
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.96	0.47
1:A:106:VAL:HG12	1:A:107:THR:N	2.29	0.47
1:A:172:LYS:HE2	1:A:180:ILE:CB	2.40	0.47
1:A:522:ILE:O	1:A:526:ILE:HG13	2.15	0.47
1:A:406:TRP:CE2	1:A:407:GLN:HG3	2.51	0.46
2:B:254:VAL:HG12	2:B:258:GLN:HE21	1.80	0.46
1:A:32:LYS:O	1:A:36:GLU:HG3	2.14	0.46
1:A:200:THR:O	1:A:203:GLU:HB3	2.16	0.46
1:A:332:GLN:OE1	1:A:332:GLN:HA	2.15	0.46
2:B:368:LEU:O	2:B:372:VAL:HG23	2.15	0.46
1:A:34:LEU:HA	1:A:37:ILE:HD12	1.97	0.46
1:A:111:VAL:N	1:A:185:ASP:O	2.49	0.46
2:B:229:TRP:CZ3	2:B:230:MET:HG2	2.50	0.46
2:B:244:ILE:HD11	2:B:427:TYR:CE2	2.51	0.46
1:A:167:ILE:HD12	1:A:212:TRP:CG	2.51	0.46
2:B:147:ASN:C	2:B:148:VAL:CG1	2.88	0.46
2:B:183:TYR:O	2:B:186:ASP:HB2	2.15	0.46
1:A:224:GLU:CB	1:A:226:PRO:CD	2.93	0.46
1:A:153:TRP:CZ3	1:A:155:GLY:HA3	2.51	0.46
1:A:537:PRO:CG	2:B:262:GLY:HA2	2.46	0.46
2:B:56:TYR:O	2:B:143:ARG:NH2	2.49	0.46
1:A:513:SER:C	1:A:515:SER:H	2.23	0.46
1:A:17:ASP:O	1:A:83:ARG:HD3	2.16	0.45
1:A:149:LEU:HD12	1:A:160:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:OD1	1:A:186:ASP:CA	2.64	0.45
2:B:357:MET:HG3	2:B:361:HIS:HD2	1.79	0.45
1:A:195:ILE:CG2	1:A:196:GLY:N	2.79	0.45
1:A:50:ILE:C	1:A:51:GLY:O	2.57	0.45
1:A:224:GLU:H	1:A:224:GLU:HG2	1.34	0.45
1:A:289:LEU:HD13	1:A:289:LEU:HA	1.60	0.45
1:A:419:THR:O	1:A:419:THR:OG1	2.34	0.45
2:B:65:LYS:O	2:B:66:LYS:C	2.58	0.45
2:B:335:GLY:HA2	2:B:367:GLN:OE1	2.17	0.45
1:A:77:PHE:O	1:A:81:ASN:ND2	2.50	0.45
1:A:84:THR:HG21	1:A:153:TRP:CZ2	2.51	0.45
1:A:288:ALA:CB	1:A:291:GLU:HB2	2.44	0.45
1:A:424:LYS:HG3	1:A:425:LEU:H	1.78	0.45
1:A:465:LYS:NZ	5:A:591:HOH:O	2.49	0.45
2:B:156:SER:HB2	2:B:157:PRO:CD	2.46	0.45
2:B:339:TYR:O	2:B:340:GLN:HG3	2.17	0.45
2:B:267:ALA:HB1	2:B:310:LEU:HD21	1.98	0.45
1:A:230:MET:HE3	1:A:230:MET:HB2	1.82	0.45
2:B:342:TYR:CD1	2:B:342:TYR:C	2.95	0.45
2:B:402:TRP:CZ2	2:B:403:THR:HG22	2.52	0.45
1:A:63:ILE:HD12	1:A:64:LYS:H	1.82	0.45
1:A:146:TYR:HB3	1:A:150:PRO:HG3	1.98	0.45
2:B:49:LYS:HG2	2:B:144:TYR:CE2	2.52	0.45
1:A:330:GLN:HE22	1:A:340:GLN:CD	2.25	0.44
2:B:27:THR:O	2:B:31:ILE:HG13	2.17	0.44
1:A:153:TRP:CD1	1:A:154:LYS:H	2.35	0.44
1:A:153:TRP:CG	1:A:154:LYS:N	2.84	0.44
2:B:150:PRO:O	2:B:156:SER:OG	2.29	0.44
2:B:390:LYS:HE2	2:B:415:GLU:OE1	2.18	0.44
1:A:21:VAL:HG12	1:A:22:LYS:N	2.32	0.44
1:A:63:ILE:CD1	1:A:64:LYS:H	2.31	0.44
1:A:329:ILE:O	1:A:392:PRO:HD3	2.17	0.44
1:A:451:LYS:HB3	1:A:471:ASN:HA	2.00	0.44
2:B:376:THR:O	2:B:380:ILE:HG13	2.18	0.44
1:A:146:TYR:CG	1:A:150:PRO:HG3	2.52	0.44
1:A:206:ARG:NE	1:A:218:ASP:OD2	2.51	0.44
1:A:311:LYS:HD2	1:A:311:LYS:HA	1.75	0.44
1:A:31:ILE:O	1:A:32:LYS:C	2.60	0.44
2:B:130:PHE:CE2	2:B:144:TYR:HB2	2.53	0.44
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.52	0.44
1:A:264:LEU:O	1:A:268:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:PHE:O	2:B:88:TRP:CD1	2.71	0.44
2:B:266:TRP:HH2	2:B:427:TYR:CE2	2.35	0.44
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.52	0.44
1:A:21:VAL:HG11	1:A:59:PRO:HD3	2.00	0.44
1:A:69:THR:HG23	1:A:69:THR:O	2.18	0.44
1:A:255:ASN:ND2	1:A:258:GLN:OE1	2.51	0.44
2:B:60:VAL:O	2:B:60:VAL:HG13	2.17	0.44
2:B:244:ILE:HD12	2:B:266:TRP:HZ3	1.83	0.44
1:A:254:VAL:HG12	1:A:254:VAL:O	2.18	0.43
1:A:334:GLN:HG3	1:A:334:GLN:O	2.18	0.43
1:A:486:LEU:HD12	1:A:521:ILE:HG23	1.99	0.43
2:B:94:ILE:HG23	2:B:95:PRO:HD2	1.99	0.43
2:B:379:SER:OG	2:B:387:PRO:HD3	2.18	0.43
1:A:187:LEU:HD12	1:A:188:TYR:N	2.33	0.43
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.48	0.43
1:A:271:TYR:CZ	1:A:314:VAL:HG23	2.53	0.43
2:B:65:LYS:HD2	2:B:72:ARG:HD2	2.00	0.43
1:A:97:PRO:HD3	1:A:232:TYR:CE1	2.53	0.43
1:A:225:PRO:CD	1:A:226:PRO:CD	2.96	0.43
1:A:195:ILE:HG23	1:A:196:GLY:N	2.31	0.43
1:A:219:LYS:H	1:A:219:LYS:HG2	1.13	0.43
2:B:138:GLU:OE1	2:B:139:THR:HG22	2.19	0.43
1:A:213:GLY:C	1:A:214:LEU:CD1	2.91	0.43
2:B:171:PHE:O	2:B:175:ASN:HB2	2.18	0.43
2:B:361:HIS:HB3	2:B:367:GLN:CD	2.44	0.43
2:B:10:VAL:HG12	2:B:11:LYS:N	2.34	0.43
1:A:21:VAL:HG13	1:A:22:LYS:N	2.34	0.43
1:A:50:ILE:HD11	1:A:143:ARG:HB3	2.01	0.43
1:A:155:GLY:O	1:A:159:ILE:HB	2.19	0.43
2:B:66:LYS:HA	2:B:66:LYS:HD3	1.86	0.43
2:B:320:ASP:HB3	2:B:323:LYS:HE2	2.01	0.43
1:A:103:LYS:HD2	1:A:103:LYS:HA	1.83	0.43
1:A:168:LEU:C	1:A:170:PRO:CD	2.92	0.43
2:B:281:LYS:HE2	2:B:284:ARG:CZ	2.49	0.43
2:B:423:VAL:HA	2:B:426:TRP:CE3	2.54	0.43
1:A:356:ARG:HD2	1:A:357:MET:O	2.19	0.42
2:B:86:ASP:HB2	2:B:88:TRP:CH2	2.54	0.42
1:A:439:THR:CG2	2:B:289:LEU:HG	2.49	0.42
2:B:74:LEU:HD12	2:B:75:VAL:N	2.34	0.42
2:B:172:LYS:O	2:B:176:PRO:HA	2.19	0.42
1:A:54:ASN:OD1	1:A:55:PRO:HD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:TYR:CB	1:A:150:PRO:HG3	2.49	0.42
1:A:297:GLU:O	1:A:297:GLU:CD	2.62	0.42
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.54	0.42
1:A:65:LYS:HA	1:A:65:LYS:CE	2.43	0.42
1:A:225:PRO:O	1:A:227:PHE:CD1	2.73	0.42
2:B:70:LYS:CE	2:B:226:PRO:HD2	2.49	0.42
1:A:117:SER:HB2	1:A:214:LEU:HG	2.00	0.42
1:A:302:GLU:C	1:A:304:ALA:N	2.74	0.42
1:A:538:ALA:N	5:A:559:HOH:O	2.52	0.42
2:B:279:LEU:O	2:B:282:LEU:HB2	2.19	0.42
1:A:495:ILE:O	1:A:495:ILE:HG22	2.19	0.42
1:A:412:PRO:O	1:A:413:GLU:C	2.62	0.42
2:B:282:LEU:HD11	2:B:299:ALA:CB	2.49	0.42
1:A:543:GLY:C	1:A:545:ASN:H	2.28	0.42
2:B:282:LEU:HD11	2:B:299:ALA:HB1	2.01	0.42
1:A:40:GLU:O	1:A:43:LYS:HB2	2.20	0.42
1:A:463:ARG:HG2	1:A:464:GLN:N	2.34	0.41
1:A:41:MET:HE2	1:A:47:ILE:HG23	2.01	0.41
1:A:136:ASN:ND2	1:A:136:ASN:C	2.73	0.41
1:A:325:LEU:HD12	1:A:325:LEU:HA	1.94	0.41
2:B:72:ARG:HG3	2:B:225:PRO:CD	2.51	0.41
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.20	0.41
1:A:215:THR:HG23	1:A:215:THR:O	2.20	0.41
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.84	0.41
1:A:439:THR:HG21	2:B:289:LEU:HG	2.02	0.41
2:B:280:SER:C	2:B:282:LEU:N	2.78	0.41
1:A:89:GLU:HB2	1:A:92:LEU:HD13	2.01	0.41
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.55	0.41
1:A:494:ASN:HB3	2:B:289:LEU:HD12	2.02	0.41
1:A:135:ILE:CD1	1:A:135:ILE:C	2.93	0.41
1:A:198:HIS:O	1:A:202:ILE:HG12	2.21	0.41
1:A:278:GLN:O	1:A:282:LEU:HD21	2.21	0.41
1:A:435:VAL:HA	2:B:290:THR:HG21	2.01	0.41
2:B:17:ASP:O	2:B:83:ARG:NH1	2.53	0.41
2:B:427:TYR:C	2:B:428:GLN:HE21	2.29	0.41
1:A:89:GLU:HB3	1:A:92:LEU:HD13	2.02	0.41
2:B:75:VAL:CG1	2:B:77:PHE:CE1	3.04	0.41
2:B:76:ASP:OD1	2:B:411:ILE:HD12	2.21	0.41
1:A:515:SER:O	1:A:519:ASN:ND2	2.53	0.41
2:B:37:ILE:O	2:B:41:MET:HG3	2.21	0.41
2:B:168:LEU:O	2:B:172:LYS:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ILE:O	2:B:206:ARG:N	2.46	0.41
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.56	0.41
1:A:44:GLU:HB3	1:A:46:LYS:HE2	2.03	0.41
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.94	0.41
1:A:377:THR:O	1:A:381:VAL:HG23	2.21	0.41
2:B:68:SER:C	2:B:70:LYS:H	2.24	0.41
2:B:197:GLN:O	2:B:201:LYS:HG2	2.20	0.41
1:A:50:ILE:HG13	1:A:143:ARG:HB2	2.02	0.40
1:A:406:TRP:CZ2	1:A:407:GLN:HG3	2.56	0.40
1:A:253:THR:CG2	1:A:256:ASP:HB2	2.41	0.40
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.61	0.40
2:B:195:ILE:O	2:B:199:ARG:HG3	2.21	0.40
1:A:21:VAL:HG13	1:A:22:LYS:H	1.87	0.40
2:B:7:THR:HG22	2:B:119:PRO:HG2	2.04	0.40
1:A:447:ASN:O	1:A:451:LYS:N	2.45	0.40
2:B:379:SER:CB	2:B:387:PRO:HD3	2.51	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	550/555 (99%)	513 (93%)	36 (6%)	1 (0%)	43	72
2	B	403/428 (94%)	370 (92%)	32 (8%)	1 (0%)	43	72
All	All	953/983 (97%)	883 (93%)	68 (7%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	152	GLY
1	A	157	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	493/495 (100%)	432 (88%)	61 (12%)	4	16
2	B	371/390 (95%)	332 (90%)	39 (10%)	6	22
All	All	864/885 (98%)	764 (88%)	100 (12%)	5	18

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	21	VAL
1	A	50	ILE
1	A	53	GLU
1	A	63	ILE
1	A	64	LYS
1	A	65	LYS
1	A	66	LYS
1	A	67	ASP
1	A	68	SER
1	A	72	ARG
1	A	73	LYS
1	A	89	GLU
1	A	90	VAL
1	A	91	GLN
1	A	92	LEU
1	A	110	ASP
1	A	116	PHE
1	A	126	LYS
1	A	135	ILE
1	A	136	ASN
1	A	137	ASN
1	A	156	SER
1	A	169	GLU
1	A	174	GLN
1	A	179	VAL
1	A	187	LEU

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Mol	Chain	Res	Type
1	A	201	LYS
1	A	219	LYS
1	A	222	GLN
1	A	248	GLU
1	A	253	THR
1	A	264	LEU
1	A	269	GLN
1	A	276	VAL
1	A	280	SER
1	A	281	LYS
1	A	282	LEU
1	A	289	LEU
1	A	291	GLU
1	A	292	VAL
1	A	296	THR
1	A	297	GLU
1	A	336	GLN
1	A	357	MET
1	A	374	LYS
1	A	376	THR
1	A	386	THR
1	A	394	GLN
1	A	411	ILE
1	A	419	THR
1	A	428	GLN
1	A	442	VAL
1	A	459	THR
1	A	480	GLN
1	A	487	GLN
1	A	497	THR
1	A	509	GLN
1	A	515	SER
1	A	517	LEU
1	A	523	GLU
2	B	8	VAL
2	B	11	LYS
2	B	16	MET
2	B	50	ILE
2	B	67	ASP
2	B	69	THR
2	B	70	LYS
2	B	82	LYS

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Mol	Chain	Res	Type
2	B	89	GLU
2	B	92	LEU
2	B	102	LYS
2	B	131	THR
2	B	138	GLU
2	B	139	THR
2	B	143	ARG
2	B	148	VAL
2	B	154	LYS
2	B	174	GLN
2	B	177	ASP
2	B	178	ILE
2	B	203	GLU
2	B	208	HIS
2	B	228	LEU
2	B	229	TRP
2	B	230	MET
2	B	240	THR
2	B	261	VAL
2	B	263	LYS
2	B	286	THR
2	B	300	GLU
2	B	311	LYS
2	B	314	VAL
2	B	329	ILE
2	B	340	GLN
2	B	357	MET
2	B	394	GLN
2	B	415	GLU
2	B	423	VAL
2	B	424	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	151	GLN
1	A	197	GLN
1	A	235	HIS
1	A	255	ASN
1	A	269	GLN
1	A	330	GLN

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Mol	Chain	Res	Type
1	A	340	GLN
1	A	394	GLN
1	A	428	GLN
1	A	474	ASN
1	A	480	GLN
1	A	487	GLN
1	A	524	GLN
2	B	137	ASN
2	B	182	GLN
2	B	208	HIS
2	B	242	GLN
2	B	258	GLN
2	B	330	GLN
2	B	340	GLN
2	B	361	HIS
2	B	394	GLN
2	B	428	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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	JTH	A	1001	4	13,13,13	1.80	3 (23%)	16,18,18	1.60	3 (18%)

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	JTH	A	1001	4	-	0/4/4/4	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	JTH	C6-C5	2.94	1.49	1.41
3	A	1001	JTH	C7-C1	2.76	1.53	1.45
3	A	1001	JTH	O1-C1	2.09	1.28	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	JTH	C5-C6-C7	3.81	132.87	130.44
3	A	1001	JTH	O1-C1-C7	2.80	122.45	116.80
3	A	1001	JTH	O7-C7-C6	2.49	120.46	116.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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 [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	552/555 (99%)	-0.03	7 (1%) 75 66	32, 88, 149, 179	0
2	B	409/428 (95%)	-0.04	5 (1%) 76 68	44, 79, 135, 166	0
All	All	961/983 (97%)	-0.03	12 (1%) 76 68	32, 84, 144, 179	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	228	LEU	3.5
1	A	257	ILE	3.4
1	A	554	ALA	3.1
2	B	360	ALA	3.0
1	A	225	PRO	2.7
1	A	541	GLY	2.7
1	A	253	THR	2.3
2	B	354	TYR	2.3
1	A	92	LEU	2.3
1	A	214	LEU	2.3
2	B	171	PHE	2.2
2	B	213	GLY	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($\text{\AA}^2$)	Q<0.9
3	JTH	A	1001	13/13	0.91	0.14	92,102,110,112	0
4	MN	A	556	1/1	0.95	0.05	60,60,60,60	0
4	MN	A	557	1/1	0.95	0.10	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.