



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:24 AM UTC

PDB ID : 2HA9 / pdb_00002ha9
Title : Crystal structure of protein SP0239 from Streptococcus pneumoniae
Authors : Chang, C.; Hatzos, C.; Abdullah, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-06-12
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

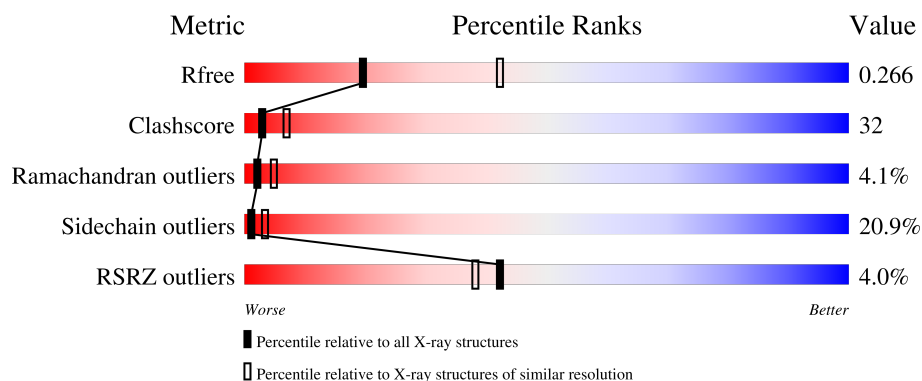
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	 4% 42% 32% 14% 7%
1	B	446	 3% 41% 33% 14% 5% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6011 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 UPF0210 protein SP0239.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	Se	0	0	0
			2978	1867	504	586	4	17			
1	B	415	Total	C	N	O	S	Se	0	0	0
			2979	1865	508	587	3	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	cloning artifact	UNP Q97ST4
A	1	MSE	MET	modified residue	UNP Q97ST4
A	12	MSE	MET	modified residue	UNP Q97ST4
A	25	MSE	MET	modified residue	UNP Q97ST4
A	158	MSE	MET	modified residue	UNP Q97ST4
A	164	MSE	MET	modified residue	UNP Q97ST4
A	177	MSE	MET	modified residue	UNP Q97ST4
A	195	MSE	MET	modified residue	UNP Q97ST4
A	255	MSE	MET	modified residue	UNP Q97ST4
A	288	MSE	MET	modified residue	UNP Q97ST4
A	315	MSE	MET	modified residue	UNP Q97ST4
A	336	MSE	MET	modified residue	UNP Q97ST4
A	353	MSE	MET	modified residue	UNP Q97ST4
A	363	MSE	MET	modified residue	UNP Q97ST4
A	378	MSE	MET	modified residue	UNP Q97ST4
A	390	MSE	MET	modified residue	UNP Q97ST4
A	406	MSE	MET	modified residue	UNP Q97ST4
A	419	MSE	MET	modified residue	UNP Q97ST4
B	0	ALA	-	cloning artifact	UNP Q97ST4
B	1	MSE	MET	modified residue	UNP Q97ST4
B	12	MSE	MET	modified residue	UNP Q97ST4
B	25	MSE	MET	modified residue	UNP Q97ST4
B	158	MSE	MET	modified residue	UNP Q97ST4
B	164	MSE	MET	modified residue	UNP Q97ST4
B	177	MSE	MET	modified residue	UNP Q97ST4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	195	MSE	MET	modified residue	UNP Q97ST4
B	255	MSE	MET	modified residue	UNP Q97ST4
B	288	MSE	MET	modified residue	UNP Q97ST4
B	315	MSE	MET	modified residue	UNP Q97ST4
B	336	MSE	MET	modified residue	UNP Q97ST4
B	353	MSE	MET	modified residue	UNP Q97ST4
B	363	MSE	MET	modified residue	UNP Q97ST4
B	378	MSE	MET	modified residue	UNP Q97ST4
B	390	MSE	MET	modified residue	UNP Q97ST4
B	406	MSE	MET	modified residue	UNP Q97ST4
B	419	MSE	MET	modified residue	UNP Q97ST4

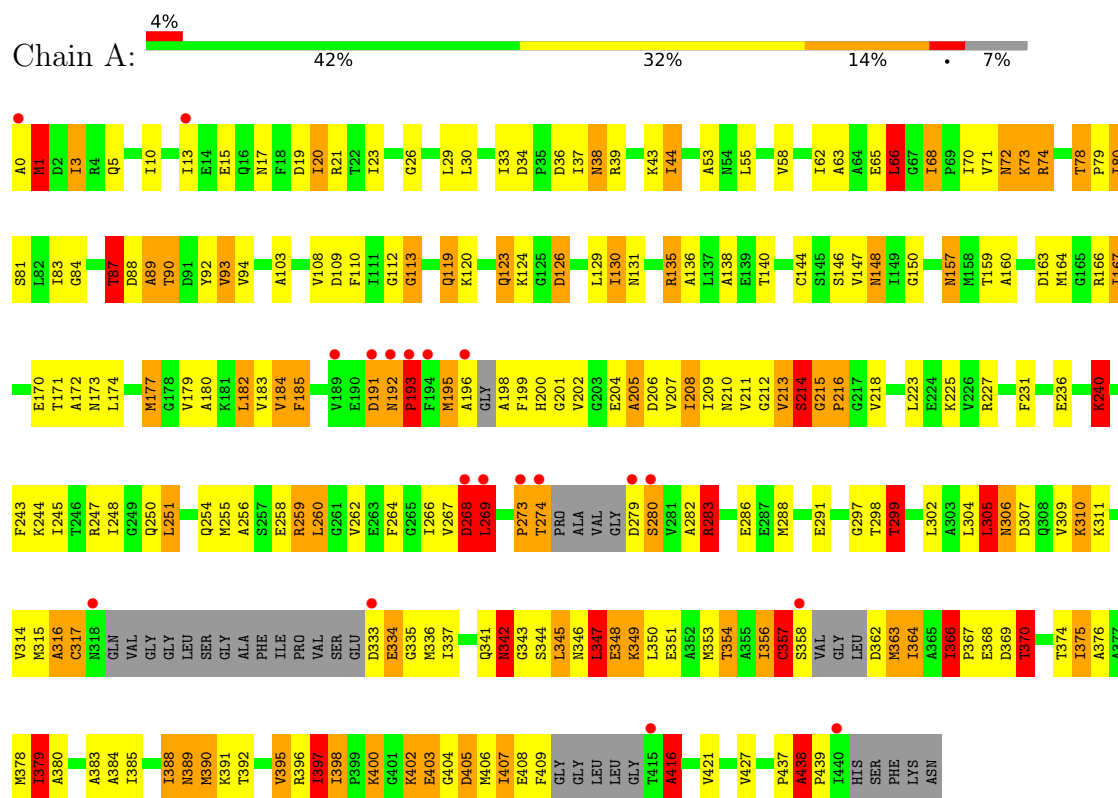
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	27	Total O 27 27	0	0
2	B	27	Total O 27 27	0	0

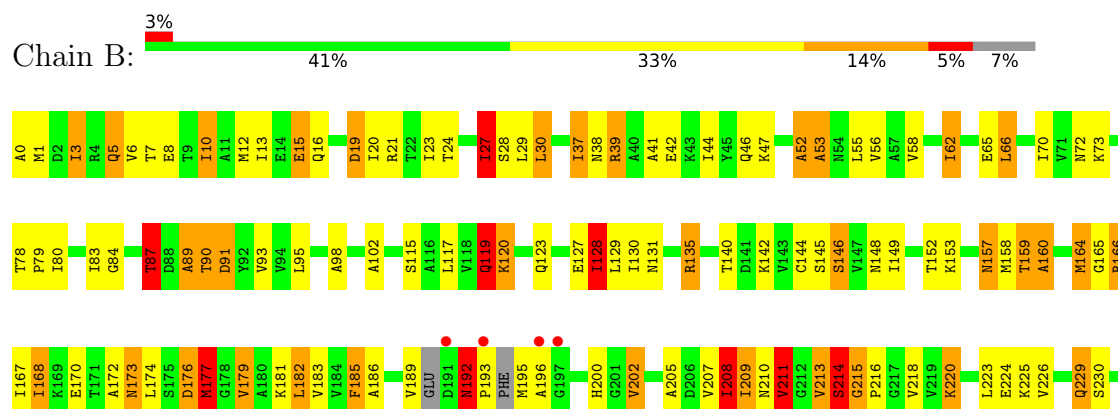
3 Residue-property plots

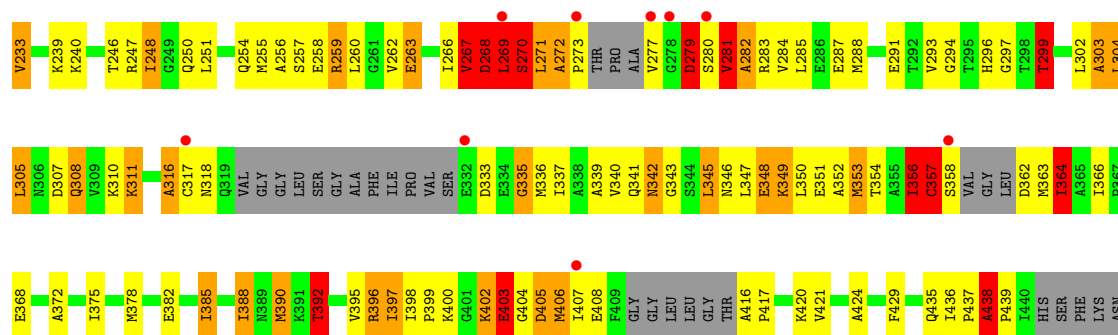
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: UPF0210 protein SP0239



• Molecule 1: UPF0210 protein SP0239





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.91Å 139.96Å 148.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.70) 95.4 (50.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.271 0.191 , 0.266	Depositor DCC
R_{free} test set	1672 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.7	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	0.95	EDS
Total number of atoms	6011	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.90	66/2982 (2.2%)	1.77	63/4004 (1.6%)
1	B	2.01	63/2982 (2.1%)	1.91	85/4002 (2.1%)
All	All	1.96	129/5964 (2.2%)	1.84	148/8006 (1.8%)

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	5
1	B	0	3
All	All	0	8

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	27	ILE	CA-CB	12.45	1.69	1.54
1	A	438	ALA	CA-C	-11.29	1.38	1.52
1	A	383	ALA	CA-CB	-11.10	1.35	1.53
1	B	438	ALA	CA-C	-9.43	1.41	1.52
1	B	438	ALA	N-CA	8.96	1.58	1.46
1	B	364	ILE	CG1-CD1	8.50	1.84	1.51
1	B	420	LYS	CA-CB	8.33	1.66	1.53
1	B	202	VAL	CA-CB	-8.19	1.43	1.54
1	A	185	PHE	CB-CG	-8.13	1.31	1.50
1	A	388	ILE	CA-CB	8.09	1.65	1.54
1	B	123	GLN	CD-NE2	8.08	1.50	1.33
1	B	177	MSE	CG-SE	7.97	2.19	1.95
1	A	44	ILE	CA-CB	-7.93	1.45	1.54
1	A	438	ALA	N-CA	7.88	1.57	1.46
1	B	186	ALA	CA-CB	-7.68	1.40	1.53
1	A	103	ALA	CA-CB	-7.68	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	ALA	CA-CB	-7.68	1.41	1.53
1	B	123	GLN	CG-CD	7.67	1.71	1.52
1	B	185	PHE	CA-C	-7.65	1.43	1.52
1	B	192	ASN	CA-C	7.61	1.62	1.52
1	A	376	ALA	CA-CB	-7.37	1.41	1.53
1	B	185	PHE	CA-CB	-7.10	1.41	1.54
1	B	269	LEU	N-CA	7.04	1.55	1.46
1	A	356	ILE	CA-CB	7.03	1.62	1.54
1	B	98	ALA	CA-CB	-7.00	1.42	1.53
1	A	173	ASN	CA-C	-6.92	1.42	1.52
1	A	298	THR	CA-CB	6.91	1.64	1.53
1	B	392	THR	C-O	-6.83	1.15	1.24
1	B	47	LYS	C-O	6.81	1.32	1.24
1	A	136	ALA	CA-CB	-6.79	1.42	1.53
1	B	269	LEU	CA-C	6.74	1.61	1.52
1	B	408	GLU	N-CA	6.70	1.54	1.46
1	B	397	ILE	CA-CB	-6.68	1.46	1.54
1	B	24	THR	C-O	-6.68	1.16	1.24
1	A	202	VAL	CA-CB	-6.60	1.47	1.54
1	B	424	ALA	C-O	-6.54	1.16	1.24
1	A	138	ALA	N-CA	6.54	1.54	1.46
1	B	267	VAL	CA-C	-6.47	1.45	1.52
1	A	23	ILE	C-O	-6.43	1.17	1.24
1	A	268	ASP	CA-C	6.41	1.61	1.52
1	B	52	ALA	CA-CB	-6.39	1.43	1.53
1	B	89	ALA	C-O	-6.38	1.16	1.24
1	A	438	ALA	CA-CB	-6.25	1.43	1.53
1	B	102	ALA	CA-CB	-6.23	1.43	1.53
1	B	248	ILE	CA-CB	-6.20	1.45	1.54
1	A	366	ILE	CA-CB	6.19	1.62	1.54
1	A	144	CYS	CA-C	-6.18	1.45	1.52
1	B	220	LYS	CD-CE	6.17	1.71	1.52
1	B	256	ALA	CA-CB	-6.14	1.43	1.53
1	B	267	VAL	C-O	-6.13	1.17	1.24
1	A	148	ASN	C-O	6.11	1.31	1.24
1	B	37	ILE	CA-CB	-6.10	1.45	1.54
1	B	281	VAL	N-CA	6.10	1.53	1.46
1	B	214	SER	C-O	6.07	1.31	1.24
1	A	316	ALA	C-O	-6.07	1.16	1.24
1	A	337	ILE	CA-CB	6.04	1.61	1.54
1	B	146	SER	CA-C	-6.04	1.45	1.52
1	B	297	GLY	C-O	-5.98	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	GLN	CD-NE2	5.95	1.45	1.33
1	B	142	LYS	N-CA	-5.95	1.38	1.46
1	B	41	ALA	CA-CB	-5.94	1.44	1.53
1	A	208	ILE	CG1-CD1	5.89	1.74	1.51
1	B	308	GLN	C-O	-5.89	1.17	1.24
1	A	416	ALA	CA-CB	5.88	1.62	1.53
1	B	185	PHE	CB-CG	-5.84	1.37	1.50
1	A	251	LEU	N-CA	-5.84	1.39	1.46
1	B	160	ALA	CA-CB	-5.81	1.44	1.53
1	A	72	ASN	CA-C	-5.81	1.45	1.52
1	B	186	ALA	C-O	5.80	1.30	1.23
1	A	73	LYS	N-CA	-5.79	1.39	1.46
1	B	177	MSE	SE-CE	5.79	2.12	1.95
1	A	199	PHE	C-O	-5.75	1.16	1.23
1	A	119	GLN	N-CA	5.74	1.53	1.46
1	B	388	ILE	C-O	-5.73	1.16	1.24
1	A	395	VAL	CA-CB	-5.70	1.47	1.54
1	A	172	ALA	C-O	5.68	1.30	1.24
1	A	150	GLY	C-O	5.66	1.29	1.23
1	A	140	THR	C-O	-5.64	1.16	1.23
1	B	211	VAL	CA-C	-5.61	1.45	1.52
1	B	19	ASP	C-O	5.61	1.30	1.23
1	A	173	ASN	N-CA	-5.58	1.38	1.46
1	A	306	ASN	N-CA	-5.58	1.39	1.46
1	A	62	ILE	CA-CB	-5.57	1.47	1.54
1	B	316	ALA	CA-CB	-5.57	1.44	1.53
1	A	251	LEU	CA-CB	-5.56	1.44	1.53
1	A	283	ARG	CZ-NH1	5.55	1.40	1.32
1	A	124	LYS	C-O	5.52	1.30	1.23
1	B	239	LYS	C-O	5.50	1.30	1.24
1	A	269	LEU	N-CA	5.49	1.53	1.46
1	A	191	ASP	CA-C	5.49	1.59	1.52
1	A	38	ASN	N-CA	5.48	1.53	1.46
1	A	174	LEU	N-CA	-5.44	1.38	1.45
1	B	372	ALA	CA-C	5.37	1.59	1.52
1	B	305	LEU	CA-C	-5.37	1.46	1.52
1	A	185	PHE	CA-CB	-5.36	1.43	1.54
1	A	347	LEU	CA-C	5.36	1.59	1.52
1	A	264	PHE	C-O	-5.34	1.17	1.23
1	A	177	MSE	CG-SE	5.31	2.11	1.95
1	A	23	ILE	CA-CB	-5.30	1.48	1.54
1	A	90	THR	N-CA	-5.29	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	LEU	CG-CD1	5.29	1.70	1.52
1	B	91	ASP	C-O	5.29	1.30	1.23
1	A	174	LEU	C-O	5.28	1.31	1.24
1	B	176	ASP	CA-C	-5.25	1.46	1.52
1	A	184	VAL	CA-CB	-5.24	1.47	1.54
1	A	375	ILE	CA-CB	-5.23	1.48	1.54
1	A	231	PHE	N-CA	-5.21	1.39	1.46
1	B	168	ILE	CA-CB	-5.20	1.48	1.54
1	B	123	GLN	CD-OE1	5.20	1.33	1.23
1	A	380	ALA	CA-CB	-5.17	1.44	1.53
1	A	112	GLY	CA-C	-5.16	1.47	1.52
1	A	205	ALA	CA-CB	-5.16	1.45	1.53
1	B	303	ALA	C-O	-5.14	1.18	1.24
1	A	354	THR	N-CA	-5.14	1.39	1.46
1	B	27	ILE	CG1-CD1	-5.14	1.31	1.51
1	B	208	ILE	N-CA	5.14	1.51	1.46
1	A	53	ALA	C-O	-5.13	1.17	1.24
1	B	233	VAL	CA-CB	5.11	1.60	1.54
1	A	146	SER	N-CA	5.10	1.52	1.46
1	A	248	ILE	CA-CB	5.07	1.60	1.54
1	B	282	ALA	CA-CB	-5.06	1.45	1.53
1	A	309	VAL	CA-CB	5.05	1.59	1.54
1	B	128	ILE	CA-CB	5.05	1.60	1.54
1	A	357	CYS	CA-C	-5.05	1.46	1.52
1	A	68	ILE	CA-C	-5.03	1.47	1.52
1	B	291	GLU	CA-C	-5.03	1.46	1.53
1	B	240	LYS	C-O	-5.01	1.18	1.24
1	A	334	GLU	N-CA	5.01	1.52	1.46
1	B	140	THR	C-O	-5.00	1.17	1.23

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	ILE	CA-C-N	-12.72	103.94	119.84
1	B	398	ILE	C-N-CA	-12.72	103.94	119.84
1	B	128	ILE	N-CA-C	-12.14	98.45	110.72
1	B	417	PRO	N-CA-CB	12.14	113.44	103.36
1	B	215	GLY	CA-C-N	10.44	132.89	119.84
1	B	215	GLY	C-N-CA	10.44	132.89	119.84
1	A	268	ASP	N-CA-C	10.20	132.53	110.80
1	B	185	PHE	CB-CA-C	-10.11	90.28	110.30
1	B	46	GLN	N-CA-C	-9.80	100.45	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	THR	N-CA-C	-9.42	101.03	114.12
1	B	208	ILE	CB-CA-C	-9.41	93.54	110.48
1	B	270	SER	N-CA-C	9.30	126.86	108.18
1	B	438	ALA	CA-C-N	9.22	149.14	127.00
1	B	438	ALA	C-N-CA	9.22	149.14	127.00
1	B	46	GLN	CA-C-N	-8.87	107.70	120.29
1	B	46	GLN	C-N-CA	-8.87	107.70	120.29
1	B	438	ALA	C-N-CD	-8.76	101.33	120.60
1	A	185	PHE	CB-CA-C	-8.61	91.14	110.07
1	A	213	VAL	CB-CA-C	-8.57	98.55	110.90
1	A	173	ASN	N-CA-CB	8.33	122.55	110.47
1	B	435	GLN	CA-C-N	-8.21	116.68	122.59
1	B	435	GLN	C-N-CA	-8.21	116.68	122.59
1	B	164	MSE	CG-SE-CE	-8.16	80.97	98.92
1	B	213	VAL	CB-CA-C	-7.80	98.69	110.55
1	B	353	MSE	CG-SE-CE	7.77	116.02	98.92
1	B	357	CYS	N-CA-C	7.70	127.20	110.80
1	A	191	ASP	N-CA-C	7.59	119.55	111.28
1	B	364	ILE	N-CA-CB	-7.54	101.95	110.99
1	A	90	THR	N-CA-CB	-7.37	100.42	110.67
1	B	72	ASN	N-CA-C	7.31	121.05	109.50
1	B	46	GLN	CA-C-O	7.24	128.30	119.97
1	A	299	THR	CB-CA-C	7.16	124.99	110.38
1	A	119	GLN	CB-CA-C	-7.14	99.39	110.81
1	A	195	MSE	CB-CA-C	-7.13	108.34	116.54
1	B	284	VAL	N-CA-CB	6.95	118.68	110.55
1	B	223	LEU	N-CA-C	6.94	118.85	111.28
1	B	268	ASP	N-CA-C	6.90	119.66	109.24
1	A	208	ILE	CG1-CB-CG2	-6.88	90.05	110.70
1	B	266	ILE	N-CA-C	6.85	118.68	108.96
1	A	389	ASN	N-CA-C	6.82	121.20	113.02
1	B	366	ILE	CA-C-N	-6.81	112.97	119.85
1	B	366	ILE	C-N-CA	-6.81	112.97	119.85
1	B	27	ILE	CA-CB-CG1	6.74	121.86	110.40
1	A	438	ALA	N-CA-C	-6.73	94.93	109.81
1	B	119	GLN	N-CA-C	6.68	119.39	111.71
1	B	416	ALA	CA-C-N	-6.65	112.61	120.13
1	B	416	ALA	C-N-CA	-6.65	112.61	120.13
1	A	379	ILE	N-CA-C	-6.65	104.04	110.42
1	A	72	ASN	N-CA-C	6.61	120.30	109.72
1	B	335	GLY	N-CA-C	-6.61	104.83	112.50
1	B	263	GLU	CB-CA-C	-6.50	97.57	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	VAL	CA-C-N	-6.45	111.13	120.29
1	A	427	VAL	C-N-CA	-6.45	111.13	120.29
1	A	305	LEU	N-CA-C	-6.40	103.92	111.03
1	A	369	ASP	N-CA-C	-6.30	105.63	113.38
1	A	438	ALA	O-C-N	6.27	128.53	121.32
1	B	39	ARG	N-CA-C	-6.25	104.46	111.28
1	B	364	ILE	N-CA-C	-6.20	99.50	108.36
1	B	438	ALA	N-CA-C	-6.19	96.14	109.81
1	B	269	LEU	N-CA-C	6.11	123.81	110.80
1	A	366	ILE	CA-C-N	-6.11	113.38	119.92
1	A	366	ILE	C-N-CA	-6.11	113.38	119.92
1	B	390	MSE	CA-CB-CG	-6.09	101.92	114.10
1	A	171	THR	N-CA-C	-6.04	104.26	111.69
1	B	144	CYS	CA-C-N	-6.04	113.33	122.81
1	B	144	CYS	C-N-CA	-6.04	113.33	122.81
1	B	281	VAL	N-CA-CB	5.94	121.03	111.23
1	B	87	THR	N-CA-CB	-5.92	101.29	110.46
1	A	185	PHE	N-CA-C	5.90	118.15	109.24
1	B	296	HIS	CA-C-N	-5.90	117.05	123.30
1	B	296	HIS	C-N-CA	-5.90	117.05	123.30
1	B	438	ALA	CA-C-O	-5.88	112.10	120.16
1	B	299	THR	CB-CA-C	5.84	121.41	109.67
1	A	93	VAL	CB-CA-C	-5.83	103.12	112.16
1	A	407	ILE	N-CA-C	5.80	121.41	109.34
1	A	126	ASP	N-CA-C	5.79	117.27	111.07
1	B	185	PHE	N-CA-C	5.79	118.21	109.41
1	A	177	MSE	CG-SE-CE	5.78	111.64	98.92
1	B	27	ILE	CB-CA-C	-5.75	102.26	110.83
1	A	317	CYS	CA-CB-SG	-5.74	101.19	114.40
1	A	193	PRO	N-CA-C	5.70	126.91	112.10
1	A	183	VAL	CB-CA-C	-5.68	102.16	110.62
1	B	357	CYS	CA-CB-SG	-5.68	101.34	114.40
1	A	182	LEU	CB-CA-C	-5.68	100.74	110.16
1	A	90	THR	N-CA-C	-5.67	106.71	113.97
1	B	159	THR	N-CA-C	-5.62	104.36	111.11
1	A	78	THR	CA-C-N	-5.61	113.92	119.93
1	A	78	THR	C-N-CA	-5.61	113.92	119.93
1	A	109	ASP	N-CA-C	-5.61	104.00	111.24
1	B	210	ASN	CA-C-N	-5.61	115.14	122.94
1	B	210	ASN	C-N-CA	-5.61	115.14	122.94
1	A	103	ALA	CA-C-N	5.61	128.11	120.54
1	A	103	ALA	C-N-CA	5.61	128.11	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	GLY	N-CA-C	5.60	123.77	112.34
1	A	310	LYS	CA-C-N	-5.59	111.82	121.66
1	A	310	LYS	C-N-CA	-5.59	111.82	121.66
1	A	44	ILE	N-CA-C	5.58	116.22	110.36
1	B	385	ILE	CB-CA-C	-5.58	104.74	111.88
1	A	269	LEU	CA-CB-CG	5.56	135.78	116.30
1	B	364	ILE	CB-CA-C	5.55	118.39	110.84
1	A	223	LEU	N-CA-C	5.50	117.28	111.28
1	B	356	ILE	CB-CA-C	-5.50	105.87	112.19
1	A	364	ILE	N-CA-C	5.49	115.77	107.80
1	B	248	ILE	CB-CA-C	-5.47	103.68	112.16
1	A	163	ASP	N-CA-C	-5.46	105.44	111.71
1	A	240	LYS	N-CA-C	5.42	117.19	111.28
1	B	208	ILE	CA-CB-CG2	5.41	119.70	110.50
1	A	398	ILE	CB-CA-C	-5.40	101.53	111.36
1	A	66	LEU	N-CA-C	-5.40	106.74	113.38
1	B	173	ASN	CB-CA-C	5.36	119.66	110.01
1	A	138	ALA	N-CA-C	5.34	117.19	111.36
1	A	349	LYS	N-CA-C	-5.34	105.37	111.14
1	B	172	ALA	CA-C-N	-5.34	112.72	122.38
1	B	172	ALA	C-N-CA	-5.34	112.72	122.38
1	B	282	ALA	N-CA-C	-5.34	105.46	111.28
1	A	317	CYS	CA-C-N	5.33	131.30	121.70
1	A	317	CYS	C-N-CA	5.33	131.30	121.70
1	B	83	ILE	N-CA-C	-5.33	105.65	110.82
1	B	388	ILE	CB-CG1-CD1	-5.31	102.66	113.80
1	B	209	ILE	CB-CG1-CD1	-5.30	102.67	113.80
1	B	281	VAL	N-CA-C	5.30	120.36	109.34
1	B	145	SER	N-CA-CB	-5.28	102.06	111.08
1	A	297	GLY	N-CA-C	-5.28	107.94	113.58
1	B	90	THR	N-CA-CB	-5.26	103.62	110.88
1	A	370	THR	CA-C-N	-5.25	114.83	120.03
1	A	370	THR	C-N-CA	-5.25	114.83	120.03
1	A	185	PHE	N-CA-CB	-5.24	102.58	111.69
1	B	230	SER	N-CA-C	5.23	116.84	110.41
1	A	3	ILE	N-CA-CB	5.21	118.40	110.58
1	B	208	ILE	N-CA-C	-5.21	100.37	108.44
1	A	214	SER	N-CA-C	5.19	121.85	110.80
1	A	291	GLU	N-CA-C	5.16	116.91	111.28
1	B	47	LYS	CA-CB-CG	-5.13	103.84	114.10
1	B	65	GLU	N-CA-C	5.13	116.87	111.28
1	B	166	ARG	NE-CZ-NH1	-5.13	116.37	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	THR	N-CA-CB	-5.12	103.33	111.62
1	B	37	ILE	CB-CA-C	-5.12	104.23	112.16
1	B	398	ILE	C-N-CD	5.11	145.96	125.00
1	B	165	GLY	N-CA-C	-5.10	106.32	112.49
1	B	280	SER	CA-C-N	5.09	131.14	121.97
1	B	280	SER	C-N-CA	5.09	131.14	121.97
1	B	258	GLU	N-CA-C	5.08	117.22	111.02
1	B	53	ALA	CA-C-N	-5.08	114.16	122.54
1	B	53	ALA	C-N-CA	-5.08	114.16	122.54
1	A	388	ILE	CB-CA-C	5.06	118.78	111.65
1	A	129	LEU	CA-CB-CG	-5.05	98.62	116.30
1	B	185	PHE	N-CA-CB	-5.01	103.47	111.43
1	A	397	ILE	CB-CA-C	-5.00	104.71	110.91

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ASN	Peptide
1	A	268	ASP	Peptide
1	A	269	LEU	Peptide
1	A	416	ALA	Peptide
1	A	437	PRO	Peptide
1	B	268	ASP	Peptide
1	B	269	LEU	Peptide
1	B	437	PRO	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	2978	0	3041	213	0
1	B	2979	0	3035	199	0
2	A	27	0	0	2	0
2	B	27	0	0	5	0
All	All	6011	0	6076	389	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (389) 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:208:ILE:CG1	1:A:208:ILE:CD1	1.74	1.60
1:B:364:ILE:CD1	1:B:364:ILE:CG1	1.84	1.50
1:B:177:MSE:SE	1:B:177:MSE:CG	2.19	1.39
1:B:251:LEU:HG	1:B:255:MSE:CE	1.68	1.22
1:A:438:ALA:HB2	1:B:311:LYS:HZ3	1.10	1.13
1:B:251:LEU:HG	1:B:255:MSE:HE2	1.18	1.11
1:B:208:ILE:HD13	1:B:208:ILE:N	1.54	1.10
1:A:177:MSE:HE2	1:A:409:PHE:CB	1.82	1.09
1:B:3:ILE:HD13	1:B:3:ILE:H	1.15	1.09
1:A:251:LEU:HD11	1:A:255:MSE:HE3	1.17	1.09
1:A:438:ALA:HB2	1:B:311:LYS:NZ	1.69	1.07
1:B:273:PRO:HD2	1:B:279:ASP:HB2	1.11	1.06
1:B:251:LEU:CG	1:B:255:MSE:HE2	1.85	1.06
1:B:349:LYS:HG3	1:B:353:MSE:CE	1.85	1.06
1:B:273:PRO:CD	1:B:279:ASP:HB2	1.84	1.05
1:B:176:ASP:O	1:B:400:LYS:HE3	1.57	1.04
1:B:375:ILE:HA	1:B:378:MSE:HE3	1.40	1.04
1:A:251:LEU:CD1	1:A:255:MSE:HE3	1.91	1.01
1:B:87:THR:HG23	1:B:89:ALA:H	1.24	1.00
1:A:349:LYS:HG3	1:A:353:MSE:HE3	1.42	0.99
1:B:349:LYS:HG3	1:B:353:MSE:HE3	1.41	0.99
1:B:375:ILE:HA	1:B:378:MSE:CE	1.93	0.97
1:A:19:ASP:CB	1:A:214:SER:HB3	1.94	0.96
1:A:438:ALA:CB	1:A:439:PRO:HA	1.96	0.96
1:A:251:LEU:HD11	1:A:255:MSE:CE	1.95	0.96
1:A:19:ASP:HB3	1:A:214:SER:HB3	1.49	0.95
1:A:342:ASN:HD21	1:A:344:SER:HB3	1.26	0.95
1:B:0:ALA:HB3	1:B:251:LEU:HD13	1.47	0.95
1:A:341:GLN:HE21	1:A:406:MSE:HE1	1.30	0.92
1:A:311:LYS:NZ	1:B:438:ALA:CB	2.33	0.91
1:A:438:ALA:CB	1:A:439:PRO:CA	2.50	0.90
1:A:71:VAL:HG12	1:A:72:ASN:ND2	1.87	0.90
1:A:311:LYS:HZ3	1:B:438:ALA:CB	1.85	0.89
1:A:130:ILE:HG22	1:A:167:ILE:HD13	1.53	0.89
1:A:374:THR:HG22	1:A:378:MSE:CE	2.03	0.89
1:A:65:GLU:OE1	1:A:259:ARG:NH2	2.06	0.88
1:A:438:ALA:HB1	1:A:439:PRO:CA	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:0:ALA:N	1:B:5:GLN:HE22	1.71	0.87
1:A:342:ASN:ND2	1:A:344:SER:HB3	1.90	0.86
1:A:273:PRO:CD	1:A:279:ASP:O	2.24	0.85
1:A:311:LYS:NZ	1:B:438:ALA:HB2	1.90	0.84
1:B:0:ALA:HB1	1:B:6:VAL:HA	1.57	0.84
1:B:66:LEU:HD21	1:B:255:MSE:HE1	1.59	0.84
1:B:251:LEU:CD1	1:B:255:MSE:HE2	2.07	0.84
1:A:438:ALA:CB	1:B:311:LYS:NZ	2.40	0.84
1:B:273:PRO:CG	1:B:277:VAL:HA	2.08	0.84
1:A:438:ALA:HB1	1:A:439:PRO:HA	1.57	0.83
1:A:342:ASN:ND2	1:A:344:SER:CB	2.41	0.83
1:B:131:ASN:HD21	1:B:166:ARG:HH22	1.24	0.83
1:A:341:GLN:HE21	1:A:406:MSE:CE	1.92	0.82
1:B:87:THR:CG2	1:B:89:ALA:H	1.91	0.82
1:B:0:ALA:N	1:B:5:GLN:NE2	2.27	0.82
1:A:438:ALA:CB	1:B:311:LYS:HZ3	1.90	0.82
1:A:349:LYS:HG3	1:A:353:MSE:CE	2.09	0.82
1:A:268:ASP:O	1:A:269:LEU:HD23	1.80	0.80
1:B:282:ALA:HB3	1:B:335:GLY:HA3	1.63	0.80
1:B:333:ASP:CB	2:B:446:HOH:O	2.27	0.80
1:A:20:ILE:CG2	1:A:70:ILE:HG12	2.12	0.79
1:A:282:ALA:O	1:A:286:GLU:HG3	1.82	0.79
1:B:3:ILE:HD13	1:B:3:ILE:N	1.97	0.79
1:A:367:PRO:O	1:A:370:THR:HG23	1.82	0.79
1:B:0:ALA:HA	1:B:5:GLN:NE2	1.98	0.79
1:A:438:ALA:HB3	1:A:439:PRO:HA	1.65	0.78
1:B:208:ILE:N	1:B:208:ILE:CD1	2.43	0.78
1:A:374:THR:HG22	1:A:378:MSE:HE1	1.65	0.78
1:B:349:LYS:O	1:B:353:MSE:HG3	1.83	0.78
1:B:349:LYS:HG3	1:B:353:MSE:HE2	1.64	0.78
1:B:3:ILE:H	1:B:3:ILE:CD1	1.92	0.78
1:B:207:VAL:HG12	1:B:262:VAL:HG13	1.65	0.78
1:A:311:LYS:HZ3	1:B:438:ALA:HB1	1.48	0.78
1:B:395:VAL:HG12	1:B:397:ILE:HG13	1.66	0.78
1:B:157:ASN:C	1:B:157:ASN:HD22	1.88	0.77
1:B:247:ARG:NH1	1:B:316:ALA:HB1	1.99	0.77
1:B:192:ASN:CB	1:B:193:PRO:HD3	2.15	0.76
1:B:208:ILE:HD13	1:B:208:ILE:H	1.49	0.76
1:A:84:GLY:O	1:A:87:THR:HB	1.85	0.76
1:B:0:ALA:CA	1:B:5:GLN:NE2	2.49	0.75
1:A:208:ILE:CD1	1:A:208:ILE:CG2	2.63	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:HIS:CE1	1:B:208:ILE:HD11	2.21	0.75
1:B:350:LEU:O	1:B:354:THR:HG23	1.85	0.75
1:B:247:ARG:HH11	1:B:250:GLN:HE22	1.33	0.75
1:A:273:PRO:HD2	1:A:279:ASP:O	1.87	0.74
1:B:342:ASN:C	1:B:342:ASN:HD22	1.94	0.74
1:A:208:ILE:CD1	1:A:208:ILE:HG21	2.18	0.73
1:B:157:ASN:HD21	1:B:159:THR:HB	1.53	0.73
1:B:207:VAL:HG12	1:B:262:VAL:CG1	2.19	0.73
1:A:131:ASN:HD21	1:A:166:ARG:HH12	1.36	0.73
1:B:56:VAL:HG13	1:B:73:LYS:CD	2.18	0.72
1:A:345:LEU:HD21	1:A:353:MSE:HE1	1.71	0.72
1:B:0:ALA:CB	1:B:251:LEU:HD13	2.19	0.72
1:A:406:MSE:SE	1:A:416:ALA:HB1	2.40	0.71
1:A:205:ALA:HB3	1:A:208:ILE:CG1	2.21	0.71
1:A:20:ILE:HG21	1:A:70:ILE:HG12	1.71	0.71
1:B:0:ALA:HA	1:B:5:GLN:CD	2.15	0.71
1:B:247:ARG:HH12	1:B:316:ALA:HB1	1.56	0.71
1:A:306:ASN:HB2	1:A:357:CYS:SG	2.31	0.70
1:A:157:ASN:C	1:A:157:ASN:HD22	1.99	0.69
1:A:208:ILE:HG21	1:A:208:ILE:HD13	1.73	0.69
1:A:346:ASN:HD22	1:B:348:GLU:HG3	1.57	0.69
1:B:362:ASP:HA	1:B:364:ILE:HD12	1.75	0.68
1:A:388:ILE:C	1:A:388:ILE:HD12	2.19	0.67
1:B:257:SER:OG	1:B:262:VAL:O	2.07	0.67
1:A:43:LYS:NZ	2:A:450:HOH:O	2.27	0.67
1:B:268:ASP:OD2	1:B:268:ASP:C	2.36	0.67
1:A:341:GLN:C	1:A:343:GLY:H	2.03	0.67
1:B:247:ARG:NH1	1:B:250:GLN:HE22	1.92	0.67
1:A:21:ARG:NH2	1:A:273:PRO:HB3	2.10	0.66
1:B:0:ALA:CB	1:B:6:VAL:HA	2.26	0.66
1:A:21:ARG:NH2	1:A:214:SER:HB2	2.10	0.66
1:A:311:LYS:HZ1	1:B:438:ALA:CB	2.09	0.66
1:B:131:ASN:ND2	1:B:166:ARG:HH22	1.94	0.66
1:A:37:ILE:HD12	1:A:87:THR:HG21	1.77	0.65
1:A:19:ASP:OD2	1:A:21:ARG:NE	2.29	0.65
1:B:0:ALA:H2	1:B:5:GLN:HE22	1.44	0.65
1:A:157:ASN:HD21	1:A:159:THR:HB	1.61	0.65
1:A:71:VAL:CG1	1:A:72:ASN:ND2	2.59	0.65
1:A:93:VAL:HG12	1:A:93:VAL:O	1.96	0.64
1:A:273:PRO:HD3	1:A:279:ASP:O	1.95	0.64
1:A:195:MSE:HA	1:A:198:ALA:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ILE:HG23	1:B:38:ASN:N	2.11	0.64
1:A:10:ILE:O	1:A:13:ILE:HG13	1.99	0.63
1:A:364:ILE:HD12	1:A:364:ILE:O	1.99	0.63
1:B:192:ASN:CB	1:B:193:PRO:CD	2.76	0.63
1:A:311:LYS:NZ	1:B:438:ALA:HB1	2.08	0.63
1:B:176:ASP:O	1:B:400:LYS:CE	2.41	0.62
1:A:195:MSE:HA	1:A:198:ALA:CB	2.28	0.62
1:A:374:THR:HG22	1:A:378:MSE:HE3	1.80	0.62
1:B:392:THR:O	1:B:392:THR:HG22	1.98	0.62
1:B:395:VAL:CG1	1:B:397:ILE:HG13	2.29	0.62
1:A:71:VAL:HG12	1:A:72:ASN:CG	2.23	0.62
1:B:273:PRO:HG2	1:B:277:VAL:HA	1.80	0.62
1:B:402:LYS:O	1:B:404:GLY:N	2.33	0.62
1:B:349:LYS:CG	1:B:353:MSE:HE3	2.23	0.62
1:A:195:MSE:O	1:A:196:ALA:HB3	1.99	0.62
1:A:84:GLY:HA3	1:A:92:TYR:CE2	2.34	0.61
1:B:273:PRO:HG3	1:B:277:VAL:HA	1.83	0.61
1:A:19:ASP:CB	1:A:214:SER:CB	2.76	0.61
1:A:311:LYS:HZ3	1:B:438:ALA:HB2	1.55	0.61
1:A:157:ASN:ND2	1:A:160:ALA:H	1.99	0.61
1:B:0:ALA:HB1	1:B:6:VAL:CA	2.29	0.61
1:A:19:ASP:HB2	1:A:214:SER:HB3	1.83	0.60
1:B:0:ALA:H1	1:B:5:GLN:HE22	1.49	0.60
1:A:208:ILE:CG2	1:A:208:ILE:HD13	2.30	0.60
1:A:1:MSE:HA	1:A:254:GLN:OE1	2.02	0.60
1:A:87:THR:CG2	1:A:89:ALA:H	2.14	0.60
1:B:56:VAL:HG13	1:B:73:LYS:HD3	1.83	0.60
1:B:157:ASN:C	1:B:157:ASN:ND2	2.55	0.60
1:A:349:LYS:CG	1:A:353:MSE:HE3	2.24	0.60
1:A:135:ARG:HH11	1:A:135:ARG:HG2	1.67	0.59
1:A:87:THR:HG23	1:A:89:ALA:H	1.66	0.59
1:A:346:ASN:HD22	1:B:348:GLU:CG	2.16	0.59
1:A:247:ARG:HH11	1:A:250:GLN:HE22	1.49	0.59
1:A:333:ASP:O	1:A:336:MSE:HB2	2.03	0.59
1:B:388:ILE:HD12	1:B:388:ILE:C	2.28	0.59
1:B:304:LEU:HD12	1:B:304:LEU:O	2.01	0.59
1:B:229:GLN:HG2	1:B:233:VAL:HG11	1.85	0.58
1:B:251:LEU:HG	1:B:255:MSE:HE1	1.77	0.58
1:B:247:ARG:HH11	1:B:250:GLN:NE2	2.01	0.58
1:A:157:ASN:C	1:A:157:ASN:ND2	2.61	0.58
1:B:37:ILE:CG2	1:B:38:ASN:N	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:0:ALA:HB1	1:B:6:VAL:HG22	1.86	0.58
1:B:362:ASP:HB2	1:B:396:ARG:HB2	1.84	0.58
1:A:131:ASN:ND2	1:A:166:ARG:HH12	2.01	0.57
1:B:368:GLU:HB2	1:B:400:LYS:HA	1.86	0.57
1:A:315:MSE:O	1:A:315:MSE:HG2	2.04	0.57
1:B:193:PRO:O	1:B:195:MSE:CB	2.52	0.57
1:A:130:ILE:HG22	1:A:167:ILE:CD1	2.32	0.57
1:B:157:ASN:ND2	1:B:160:ALA:H	2.02	0.57
1:B:207:VAL:C	1:B:208:ILE:HD13	2.27	0.57
1:B:287:GLU:HG3	1:B:287:GLU:O	2.03	0.57
1:A:438:ALA:HB3	1:A:439:PRO:CA	2.28	0.57
1:B:345:LEU:HD23	1:B:346:ASN:H	1.69	0.57
1:B:375:ILE:HA	1:B:378:MSE:HE2	1.85	0.57
1:A:135:ARG:HH11	1:A:135:ARG:CG	2.18	0.57
1:A:374:THR:CG2	1:A:378:MSE:CE	2.80	0.57
1:A:438:ALA:HB2	1:B:311:LYS:HZ1	1.68	0.57
1:B:56:VAL:HG13	1:B:73:LYS:HD2	1.86	0.57
1:B:268:ASP:OD2	1:B:268:ASP:O	2.23	0.57
1:B:20:ILE:HB	1:B:70:ILE:HG12	1.86	0.56
1:A:93:VAL:O	1:A:93:VAL:CG1	2.51	0.56
1:A:177:MSE:HE3	1:A:180:ALA:HB2	1.86	0.56
1:B:19:ASP:OD2	1:B:214:SER:HB3	2.05	0.56
1:A:130:ILE:HD12	1:A:164:MSE:HE1	1.87	0.56
1:A:438:ALA:CB	1:B:311:LYS:HZ1	2.17	0.56
1:A:251:LEU:HD21	1:A:255:MSE:HE1	1.87	0.56
1:B:119:GLN:CD	1:B:119:GLN:H	2.15	0.55
1:B:91:ASP:HA	1:B:128:ILE:HG23	1.89	0.55
1:A:200:HIS:CE1	1:A:204:GLU:HB3	2.41	0.55
1:A:227:ARG:HG3	1:A:227:ARG:HH11	1.71	0.55
1:A:307:ASP:OD2	1:B:439:PRO:HA	2.07	0.55
1:A:19:ASP:HB2	1:A:214:SER:CB	2.37	0.55
1:A:36:ASP:CG	1:A:39:ARG:HG3	2.32	0.54
1:A:341:GLN:C	1:A:343:GLY:N	2.65	0.54
1:A:342:ASN:ND2	1:A:344:SER:HB2	2.21	0.54
1:B:84:GLY:O	1:B:87:THR:HB	2.08	0.54
1:A:438:ALA:HB1	1:A:439:PRO:C	2.32	0.54
1:A:195:MSE:CA	1:A:198:ALA:HB2	2.37	0.54
1:A:366:ILE:CD1	1:A:397:ILE:CG2	2.86	0.54
1:A:73:LYS:C	1:A:74:ARG:HG2	2.32	0.54
1:A:363:MSE:SE	1:A:396:ARG:HH11	2.41	0.54
1:A:0:ALA:N	1:A:251:LEU:HD13	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ASP:CG	1:B:214:SER:HB3	2.34	0.54
1:B:196:ALA:HB1	1:B:396:ARG:HH12	1.73	0.54
1:B:307:ASP:O	1:B:311:LYS:HG2	2.08	0.54
1:A:66:LEU:HD21	1:A:255:MSE:SE	2.58	0.53
1:B:66:LEU:HD21	1:B:255:MSE:CE	2.34	0.53
1:B:304:LEU:HD12	1:B:304:LEU:C	2.32	0.53
1:A:130:ILE:CG2	1:A:167:ILE:HD13	2.31	0.53
1:B:29:LEU:HD13	1:B:44:ILE:HG12	1.91	0.53
1:B:196:ALA:CB	1:B:396:ARG:HH12	2.21	0.53
1:A:404:GLY:O	1:A:405:ASP:O	2.27	0.53
1:A:356:ILE:HG22	1:B:388:ILE:HG12	1.90	0.53
1:B:182:LEU:O	1:B:396:ARG:HG2	2.09	0.53
1:A:126:ASP:O	1:A:130:ILE:HG12	2.08	0.53
1:B:29:LEU:O	1:B:30:LEU:C	2.50	0.53
1:A:205:ALA:HB3	1:A:208:ILE:HG13	1.90	0.52
1:A:356:ILE:HG22	1:B:388:ILE:CG1	2.39	0.52
1:A:240:LYS:HD2	1:A:244:LYS:HE3	1.92	0.52
1:A:368:GLU:O	1:A:368:GLU:CG	2.56	0.52
1:A:304:LEU:HD13	1:B:436:ILE:HG23	1.91	0.52
1:B:153:LYS:O	1:B:153:LYS:HG2	2.10	0.52
1:B:247:ARG:NH1	1:B:316:ALA:CB	2.72	0.52
1:B:56:VAL:HA	1:B:73:LYS:HD3	1.91	0.52
1:A:395:VAL:HG11	1:A:397:ILE:HD11	1.91	0.52
1:B:87:THR:CG2	1:B:89:ALA:N	2.67	0.52
1:B:403:GLU:OE1	1:B:403:GLU:O	2.28	0.52
1:A:195:MSE:HG3	1:A:196:ALA:N	2.24	0.52
1:A:375:ILE:O	1:A:379:ILE:HG13	2.10	0.51
1:B:149:ILE:C	1:B:149:ILE:HD12	2.35	0.51
1:A:243:PHE:CE1	1:A:315:MSE:O	2.64	0.51
1:A:71:VAL:HG12	1:A:72:ASN:HD21	1.73	0.51
1:A:215:GLY:O	1:A:216:PRO:C	2.52	0.51
1:B:127:GLU:HB2	2:B:451:HOH:O	2.10	0.51
1:A:282:ALA:HB3	1:A:335:GLY:HA3	1.93	0.51
1:A:389:ASN:C	1:A:390:MSE:CG	2.81	0.51
1:A:131:ASN:ND2	1:A:166:ARG:NH1	2.60	0.50
1:B:164:MSE:O	1:B:168:ILE:HD12	2.11	0.50
1:A:299:THR:HG21	1:B:351:GLU:OE2	2.11	0.50
1:B:120:LYS:HG3	2:B:470:HOH:O	2.11	0.50
1:A:29:LEU:HD13	1:A:44:ILE:HD13	1.94	0.50
1:A:402:LYS:O	1:A:403:GLU:C	2.55	0.49
1:A:0:ALA:H1	1:A:251:LEU:HD13	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASN:HA	1:B:185:PHE:HB2	1.94	0.49
1:A:346:ASN:HB3	1:A:349:LYS:H	1.76	0.49
1:A:366:ILE:HD13	1:A:397:ILE:HG22	1.95	0.49
1:B:117:LEU:HD13	1:B:189:VAL:HG23	1.95	0.49
1:A:87:THR:CG2	1:A:88:ASP:N	2.75	0.49
1:B:362:ASP:O	1:B:363:MSE:HB2	2.13	0.49
1:A:0:ALA:H1	1:A:251:LEU:CD1	2.26	0.48
1:A:36:ASP:OD2	1:A:39:ARG:HG3	2.13	0.48
1:A:389:ASN:C	1:A:390:MSE:HG3	2.39	0.48
1:B:12:MSE:HA	1:B:15:GLU:OE2	2.13	0.48
1:B:226:VAL:O	1:B:229:GLN:HB2	2.12	0.48
1:B:115:SER:HB3	1:B:146:SER:O	2.13	0.48
1:A:212:GLY:HA2	1:A:268:ASP:HB2	1.96	0.48
1:A:273:PRO:HG2	1:A:279:ASP:N	2.29	0.48
1:A:191:ASP:O	1:A:192:ASN:C	2.57	0.48
1:A:201:GLY:O	1:A:204:GLU:HB2	2.13	0.48
1:A:205:ALA:HB3	1:A:208:ILE:HG12	1.96	0.48
1:B:0:ALA:H1	1:B:5:GLN:NE2	2.07	0.48
1:A:402:LYS:O	1:A:404:GLY:N	2.47	0.47
1:A:273:PRO:HB2	1:A:274:THR:H	1.29	0.47
1:A:342:ASN:HD22	1:A:344:SER:CB	2.27	0.47
1:B:341:GLN:C	1:B:343:GLY:H	2.21	0.47
1:A:251:LEU:CG	1:A:255:MSE:HE3	2.43	0.47
1:B:78:THR:O	1:B:79:PRO:C	2.56	0.47
1:B:336:MSE:O	1:B:340:VAL:HG23	2.14	0.47
1:A:388:ILE:HD12	1:A:389:ASN:N	2.30	0.47
1:A:58:VAL:HG11	1:A:260:LEU:HD22	1.97	0.47
1:B:250:GLN:HE22	1:B:316:ALA:HB1	1.80	0.47
1:A:80:ILE:O	1:A:81:SER:C	2.56	0.47
1:B:170:GLU:O	1:B:174:LEU:HB2	2.15	0.47
1:B:375:ILE:CA	1:B:378:MSE:CE	2.82	0.47
1:A:63:ALA:HB2	1:A:70:ILE:HD12	1.96	0.46
1:A:208:ILE:CD1	1:A:208:ILE:CB	2.78	0.46
1:B:272:ALA:HB2	1:B:281:VAL:HG23	1.97	0.46
1:B:30:LEU:HD13	1:B:78:THR:HG21	1.97	0.46
1:B:211:VAL:O	1:B:267:VAL:HA	2.15	0.46
1:B:346:ASN:OD1	1:B:348:GLU:OE2	2.32	0.46
1:A:280:SER:H	1:A:283:ARG:HG3	1.80	0.46
1:A:20:ILE:CB	1:A:70:ILE:HG12	2.46	0.46
1:A:193:PRO:HG2	1:A:210:ASN:HD22	1.80	0.46
1:A:244:LYS:O	1:A:245:ILE:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:CYS:HB3	1:A:358:SER:H	1.27	0.46
1:B:285:LEU:O	1:B:288:MSE:HB2	2.16	0.46
1:A:302:LEU:HB3	1:A:356:ILE:HD11	1.97	0.46
1:A:26:GLY:O	1:A:207:VAL:HA	2.15	0.46
1:A:126:ASP:O	1:A:130:ILE:CG1	2.64	0.46
1:B:382:GLU:HG3	1:B:395:VAL:HG22	1.98	0.46
1:A:84:GLY:HA3	1:A:92:TYR:CD2	2.51	0.46
1:A:195:MSE:CG	1:A:196:ALA:H	2.28	0.45
1:B:27:ILE:HG22	1:B:28:SER:O	2.16	0.45
1:B:273:PRO:HG2	1:B:277:VAL:CA	2.45	0.45
1:A:184:VAL:HG12	1:A:185:PHE:N	2.32	0.45
1:A:74:ARG:HH21	1:A:195:MSE:CB	2.29	0.45
1:A:366:ILE:HD13	1:A:397:ILE:CG2	2.47	0.45
1:A:363:MSE:SE	1:A:396:ARG:HD2	2.67	0.45
1:B:246:THR:O	1:B:250:GLN:HG3	2.17	0.45
1:B:177:MSE:HE3	1:B:181:LYS:HD3	1.99	0.44
1:A:21:ARG:HG3	1:A:21:ARG:HH11	1.80	0.44
1:A:71:VAL:CG1	1:A:72:ASN:HD21	2.29	0.44
1:A:195:MSE:O	1:A:196:ALA:CB	2.65	0.44
1:B:10:ILE:HG21	1:B:10:ILE:HD12	1.47	0.44
1:A:130:ILE:HG21	1:A:164:MSE:HE1	2.00	0.44
1:B:80:ILE:HD13	1:B:80:ILE:HA	1.77	0.44
1:B:93:VAL:HG21	1:B:135:ARG:HE	1.82	0.44
1:B:294:GLY:O	1:B:349:LYS:HE3	2.18	0.44
1:B:229:GLN:HG2	1:B:233:VAL:HG21	2.00	0.43
1:B:37:ILE:HD12	1:B:87:THR:HG21	1.99	0.43
1:B:293:VAL:CG1	1:B:339:ALA:CB	2.96	0.43
1:B:58:VAL:O	1:B:62:ILE:HG13	2.18	0.43
1:B:23:ILE:HD13	1:B:23:ILE:HG21	1.73	0.43
1:B:304:LEU:HD12	1:B:308:GLN:HG2	2.00	0.43
1:A:21:ARG:NH1	1:A:214:SER:HA	2.34	0.43
1:A:79:PRO:HA	1:A:113:GLY:O	2.19	0.43
1:B:158:MSE:O	1:B:159:THR:C	2.57	0.43
1:B:390:MSE:H	1:B:390:MSE:HG3	1.60	0.43
1:A:147:VAL:HG11	1:A:164:MSE:HE3	2.00	0.43
1:A:341:GLN:NE2	1:A:406:MSE:HE1	2.14	0.43
1:A:368:GLU:O	1:A:368:GLU:HG2	2.18	0.43
1:B:259:ARG:H	1:B:259:ARG:HG2	1.53	0.43
1:A:73:LYS:O	1:A:108:VAL:HB	2.19	0.43
1:A:87:THR:CG2	1:A:89:ALA:N	2.80	0.43
1:A:131:ASN:HD21	1:A:166:ARG:NH1	2.09	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ALA:O	1:A:385:ILE:C	2.61	0.43
1:B:3:ILE:N	1:B:3:ILE:CD1	2.67	0.43
1:B:202:VAL:H	1:B:202:VAL:HG23	1.43	0.43
1:A:299:THR:HG22	1:A:349:LYS:NZ	2.34	0.42
1:B:215:GLY:O	1:B:218:VAL:HB	2.19	0.42
1:A:78:THR:O	1:A:79:PRO:C	2.62	0.42
1:A:83:ILE:O	1:A:84:GLY:C	2.61	0.42
1:A:148:ASN:HA	1:A:185:PHE:HB2	2.01	0.42
1:A:130:ILE:CG2	1:A:164:MSE:HE1	2.49	0.42
1:A:306:ASN:CB	1:A:357:CYS:SG	3.06	0.42
1:A:255:MSE:O	1:A:256:ALA:C	2.62	0.42
1:B:149:ILE:HG13	1:B:185:PHE:O	2.19	0.42
1:B:348:GLU:CD	1:B:348:GLU:H	2.27	0.42
1:A:243:PHE:CD1	1:A:315:MSE:O	2.73	0.42
1:B:215:GLY:HA3	1:B:216:PRO:HD3	1.83	0.42
1:A:37:ILE:HG23	1:A:38:ASN:N	2.35	0.42
1:B:157:ASN:HD22	1:B:158:MSE:N	2.14	0.42
1:B:273:PRO:CD	1:B:279:ASP:CB	2.77	0.42
1:B:308:GLN:HA	1:B:311:LYS:HG3	2.02	0.42
1:A:195:MSE:HG3	1:A:196:ALA:H	1.83	0.42
1:B:193:PRO:C	1:B:195:MSE:CB	2.93	0.42
1:B:375:ILE:HG12	1:B:378:MSE:HE1	2.02	0.42
1:A:398:ILE:HG22	1:A:400:LYS:HG3	2.02	0.42
1:B:152:THR:HG21	1:B:390:MSE:HG2	2.02	0.42
1:B:282:ALA:CB	1:B:335:GLY:HA3	2.41	0.42
1:A:346:ASN:O	1:A:347:LEU:C	2.62	0.41
1:B:0:ALA:CA	1:B:5:GLN:CD	2.88	0.41
1:B:303:ALA:N	1:B:356:ILE:HD13	2.35	0.41
1:B:345:LEU:HD21	1:B:353:MSE:CE	2.50	0.41
1:A:94:VAL:HG12	2:A:455:HOH:O	2.20	0.41
1:A:266:ILE:C	1:A:266:ILE:HD12	2.45	0.41
1:A:350:LEU:O	1:A:354:THR:HG23	2.19	0.41
1:A:135:ARG:HG2	1:A:135:ARG:NH1	2.32	0.41
1:A:193:PRO:HG2	1:A:210:ASN:ND2	2.36	0.41
1:A:299:THR:CG2	1:B:351:GLU:OE2	2.67	0.41
1:A:351:GLU:OE2	1:B:299:THR:HG21	2.19	0.41
1:B:10:ILE:HA	1:B:13:ILE:HG12	2.03	0.41
1:B:179:VAL:HG22	2:B:471:HOH:O	2.19	0.41
1:A:341:GLN:O	1:A:343:GLY:N	2.53	0.41
1:A:37:ILE:CD1	1:A:87:THR:HG21	2.47	0.41
1:A:268:ASP:HB3	1:A:269:LEU:H	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASN:HD21	1:B:346:ASN:HD21	1.67	0.41
1:A:74:ARG:HH11	1:A:74:ARG:HD3	1.70	0.41
1:A:206:ASP:O	1:A:207:VAL:HG23	2.20	0.41
1:A:348:GLU:CD	1:A:348:GLU:H	2.28	0.41
1:B:129:LEU:O	1:B:129:LEU:HG	2.11	0.41
1:B:349:LYS:O	1:B:352:ALA:HB3	2.21	0.41
1:B:405:ASP:O	1:B:406:MSE:HG2	2.21	0.41
1:A:204:GLU:OE1	1:A:208:ILE:HD12	2.21	0.41
1:A:123:GLN:NE2	1:A:123:GLN:HA	2.35	0.41
1:B:270:SER:O	1:B:270:SER:OG	2.30	0.41
1:B:341:GLN:C	1:B:343:GLY:N	2.78	0.41
1:B:356:ILE:O	1:B:357:CYS:HB2	2.21	0.41
1:A:72:ASN:C	1:A:73:LYS:HG3	2.47	0.40
1:B:52:ALA:O	1:B:53:ALA:C	2.63	0.40
1:B:56:VAL:H	1:B:56:VAL:HG23	1.65	0.40
1:B:302:LEU:HD23	1:B:356:ILE:HD11	2.03	0.40
1:A:33:ILE:CG2	1:A:34:ASP:N	2.84	0.40
1:A:74:ARG:HH21	1:A:195:MSE:HB2	1.86	0.40
1:A:74:ARG:HD2	1:A:110:PHE:HB2	2.02	0.40
1:A:288:MSE:HE1	1:A:305:LEU:HB2	2.03	0.40
1:B:21:ARG:NH2	1:B:271:LEU:C	2.79	0.40
1:B:95:LEU:HD23	1:B:95:LEU:HA	1.82	0.40
1:B:128:ILE:HD13	2:B:460:HOH:O	2.22	0.40
1:B:130:ILE:HD13	1:B:164:MSE:HE1	2.03	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	402/446 (90%)	356 (89%)	31 (8%)	15 (4%)	2 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	401/446 (90%)	357 (89%)	26 (6%)	18 (4%)	2	4
All	All	803/892 (90%)	713 (89%)	57 (7%)	33 (4%)	2	5

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	PRO
1	A	214	SER
1	A	273	PRO
1	A	403	GLU
1	A	405	ASP
1	A	407	ILE
1	A	416	ALA
1	A	438	ALA
1	B	192	ASN
1	B	214	SER
1	B	269	LEU
1	B	279	ASP
1	B	317	CYS
1	B	357	CYS
1	B	403	GLU
1	B	405	ASP
1	B	406	MSE
1	B	407	ILE
1	B	438	ALA
1	A	316	ALA
1	A	342	ASN
1	A	357	CYS
1	B	205	ALA
1	B	271	LEU
1	A	1	MSE
1	A	89	ALA
1	B	429	PHE
1	B	399	PRO
1	A	317	CYS
1	B	272	ALA
1	B	318	ASN
1	A	113	GLY
1	B	281	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/329 (94%)	246 (79%)	64 (21%)	1	3
1	B	308/329 (94%)	243 (79%)	65 (21%)	1	3
All	All	618/658 (94%)	489 (79%)	129 (21%)	1	3

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	3	ILE
1	A	5	GLN
1	A	15	GLU
1	A	17	ASN
1	A	20	ILE
1	A	30	LEU
1	A	55	LEU
1	A	66	LEU
1	A	68	ILE
1	A	74	ARG
1	A	80	ILE
1	A	87	THR
1	A	90	THR
1	A	119	GLN
1	A	120	LYS
1	A	130	ILE
1	A	135	ARG
1	A	157	ASN
1	A	167	ILE
1	A	170	GLU
1	A	179	VAL
1	A	182	LEU
1	A	193	PRO
1	A	209	ILE
1	A	211	VAL
1	A	213	VAL

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Mol	Chain	Res	Type
1	A	216	PRO
1	A	218	VAL
1	A	225	LYS
1	A	236	GLU
1	A	240	LYS
1	A	258	GLU
1	A	259	ARG
1	A	260	LEU
1	A	262	VAL
1	A	267	VAL
1	A	269	LEU
1	A	274	THR
1	A	280	SER
1	A	283	ARG
1	A	299	THR
1	A	305	LEU
1	A	310	LYS
1	A	314	VAL
1	A	334	GLU
1	A	342	ASN
1	A	345	LEU
1	A	347	LEU
1	A	348	GLU
1	A	357	CYS
1	A	362	ASP
1	A	363	MSE
1	A	366	ILE
1	A	370	THR
1	A	379	ILE
1	A	390	MSE
1	A	391	LYS
1	A	392	THR
1	A	397	ILE
1	A	400	LYS
1	A	402	LYS
1	A	408	GLU
1	A	421	VAL
1	B	1	MSE
1	B	3	ILE
1	B	5	GLN
1	B	7	THR
1	B	8	GLU

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Mol	Chain	Res	Type
1	B	10	ILE
1	B	15	GLU
1	B	16	GLN
1	B	27	ILE
1	B	30	LEU
1	B	39	ARG
1	B	42	GLU
1	B	55	LEU
1	B	62	ILE
1	B	66	LEU
1	B	87	THR
1	B	90	THR
1	B	119	GLN
1	B	120	LYS
1	B	128	ILE
1	B	135	ARG
1	B	157	ASN
1	B	167	ILE
1	B	173	ASN
1	B	177	MSE
1	B	179	VAL
1	B	182	LEU
1	B	183	VAL
1	B	208	ILE
1	B	209	ILE
1	B	211	VAL
1	B	213	VAL
1	B	220	LYS
1	B	224	GLU
1	B	225	LYS
1	B	229	GLN
1	B	248	ILE
1	B	254	GLN
1	B	259	ARG
1	B	260	LEU
1	B	263	GLU
1	B	267	VAL
1	B	270	SER
1	B	279	ASP
1	B	283	ARG
1	B	299	THR
1	B	304	LEU

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Mol	Chain	Res	Type
1	B	305	LEU
1	B	310	LYS
1	B	311	LYS
1	B	337	ILE
1	B	342	ASN
1	B	345	LEU
1	B	347	LEU
1	B	348	GLU
1	B	349	LYS
1	B	356	ILE
1	B	358	SER
1	B	364	ILE
1	B	385	ILE
1	B	392	THR
1	B	396	ARG
1	B	402	LYS
1	B	403	GLU
1	B	421	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	72	ASN
1	A	131	ASN
1	A	157	ASN
1	A	229	GLN
1	A	250	GLN
1	A	308	GLN
1	A	341	GLN
1	A	342	ASN
1	A	346	ASN
1	A	389	ASN
1	B	5	GLN
1	B	16	GLN
1	B	46	GLN
1	B	72	ASN
1	B	131	ASN
1	B	157	ASN
1	B	200	HIS
1	B	250	GLN
1	B	308	GLN

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Mol	Chain	Res	Type
1	B	342	ASN
1	B	389	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	397/446 (89%)	-0.26	19 (4%) 35 32	23, 40, 74, 93	0
1	B	398/446 (89%)	-0.34	13 (3%) 49 45	22, 37, 71, 86	0
All	All	795/892 (89%)	-0.30	32 (4%) 42 38	22, 39, 72, 93	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	ALA	5.8
1	A	318	ASN	5.4
1	A	274	THR	5.2
1	A	358	SER	5.2
1	A	196	ALA	4.9
1	A	279	ASP	4.9
1	A	415	THR	4.6
1	B	191	ASP	4.5
1	B	193	PRO	3.8
1	A	193	PRO	3.7
1	B	317	CYS	3.6
1	A	269	LEU	3.6
1	B	269	LEU	3.5
1	B	277	VAL	3.4
1	A	333	ASP	3.3
1	A	440	ILE	3.1
1	A	191	ASP	2.7
1	A	194	PHE	2.7
1	B	407	ILE	2.6
1	B	278	GLY	2.6
1	B	273	PRO	2.6
1	A	273	PRO	2.5
1	A	13	ILE	2.3
1	B	332	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	268	ASP	2.2
1	B	358	SER	2.2
1	A	192	ASN	2.2
1	A	280	SER	2.1
1	B	197	GLY	2.1
1	B	196	ALA	2.0
1	B	280	SER	2.0
1	A	189	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.