



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:30 AM UTC

PDB ID : 2HFB / pdb_00002hfb
Title : Crystal structure of selenomethionine-labelled RafE from *Streptococcus pneumoniae*
Authors : Paterson, N.G.; Riboldi-Tunncliffe, A.; Mitchell, T.J.; Isaacs, N.W.
Deposited on : 2006-06-23
Resolution : 2.90 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

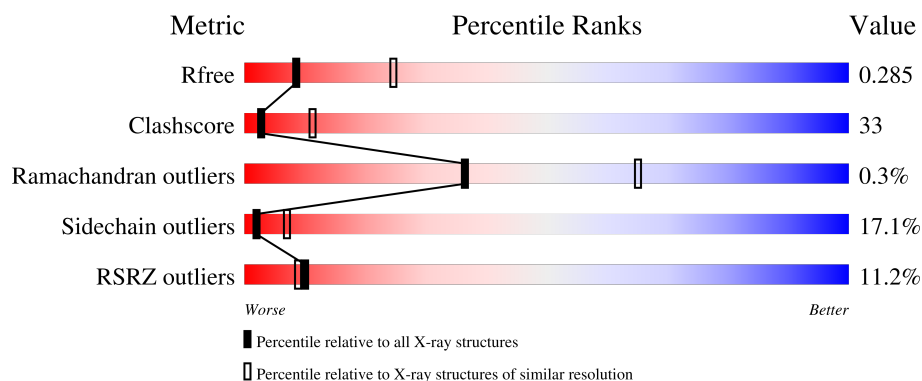
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	409	
1	B	409	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6045 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 Sugar ABC transporter, sugar-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	Se	69	0	0
			3029	1937	497	584	11			
1	B	381	Total	C	N	O	Se	376	0	0
			3013	1927	494	581	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	cloning artifact	UNP Q97NW2
A	-16	ARG	-	cloning artifact	UNP Q97NW2
A	-15	GLY	-	cloning artifact	UNP Q97NW2
A	-14	SER	-	cloning artifact	UNP Q97NW2
A	-13	HIS	-	cloning artifact	UNP Q97NW2
A	-12	HIS	-	cloning artifact	UNP Q97NW2
A	-11	HIS	-	cloning artifact	UNP Q97NW2
A	-10	HIS	-	cloning artifact	UNP Q97NW2
A	-9	HIS	-	cloning artifact	UNP Q97NW2
A	-8	HIS	-	cloning artifact	UNP Q97NW2
A	-7	THR	-	cloning artifact	UNP Q97NW2
A	-6	ASP	-	cloning artifact	UNP Q97NW2
A	-5	PRO	-	cloning artifact	UNP Q97NW2
A	17	MSE	MET	modified residue	UNP Q97NW2
A	201	MSE	MET	modified residue	UNP Q97NW2
A	208	MSE	MET	modified residue	UNP Q97NW2
A	240	MSE	MET	modified residue	UNP Q97NW2
A	264	MSE	MET	modified residue	UNP Q97NW2
A	302	MSE	MET	modified residue	UNP Q97NW2
A	308	MSE	MET	modified residue	UNP Q97NW2
A	336	MSE	MET	modified residue	UNP Q97NW2
A	364	MSE	MET	modified residue	UNP Q97NW2
A	375	MSE	MET	modified residue	UNP Q97NW2
A	386	MSE	MET	modified residue	UNP Q97NW2
B	-17	MET	-	cloning artifact	UNP Q97NW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	ARG	-	cloning artifact	UNP Q97NW2
B	-15	GLY	-	cloning artifact	UNP Q97NW2
B	-14	SER	-	cloning artifact	UNP Q97NW2
B	-13	HIS	-	cloning artifact	UNP Q97NW2
B	-12	HIS	-	cloning artifact	UNP Q97NW2
B	-11	HIS	-	cloning artifact	UNP Q97NW2
B	-10	HIS	-	cloning artifact	UNP Q97NW2
B	-9	HIS	-	cloning artifact	UNP Q97NW2
B	-8	HIS	-	cloning artifact	UNP Q97NW2
B	-7	THR	-	cloning artifact	UNP Q97NW2
B	-6	ASP	-	cloning artifact	UNP Q97NW2
B	-5	PRO	-	cloning artifact	UNP Q97NW2
B	17	MSE	MET	modified residue	UNP Q97NW2
B	201	MSE	MET	modified residue	UNP Q97NW2
B	208	MSE	MET	modified residue	UNP Q97NW2
B	240	MSE	MET	modified residue	UNP Q97NW2
B	264	MSE	MET	modified residue	UNP Q97NW2
B	302	MSE	MET	modified residue	UNP Q97NW2
B	308	MSE	MET	modified residue	UNP Q97NW2
B	336	MSE	MET	modified residue	UNP Q97NW2
B	364	MSE	MET	modified residue	UNP Q97NW2
B	375	MSE	MET	modified residue	UNP Q97NW2
B	386	MSE	MET	modified residue	UNP Q97NW2

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

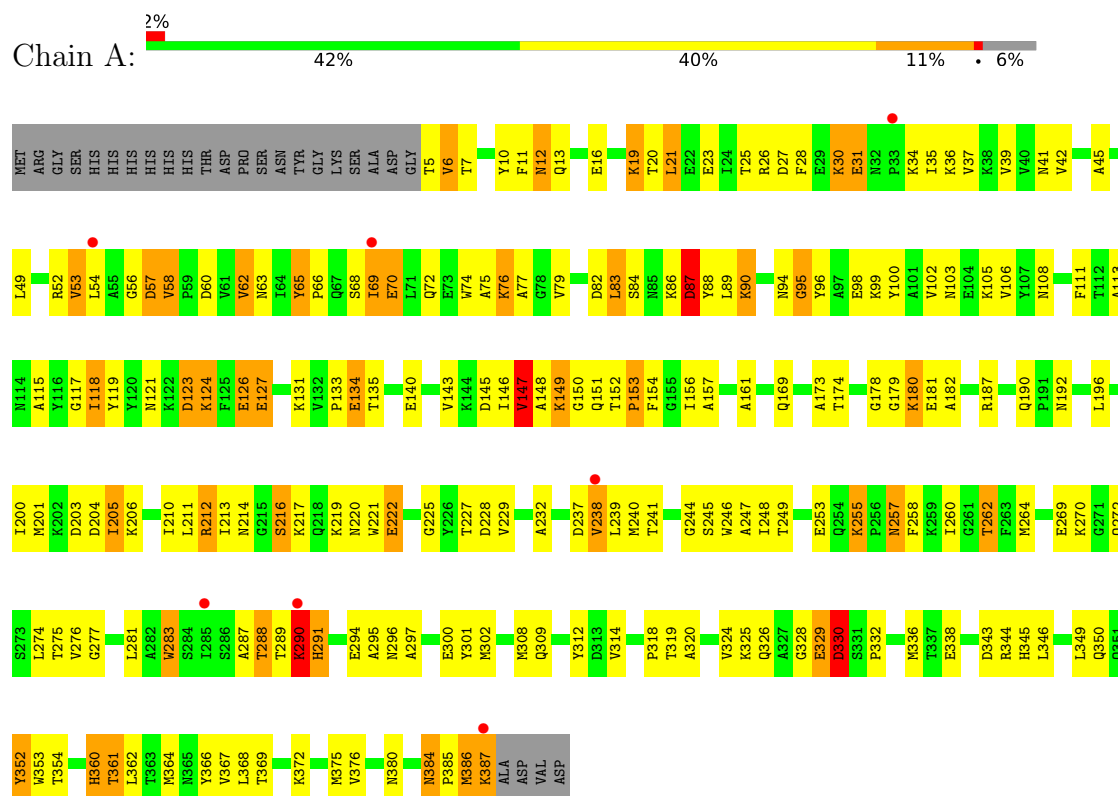
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0

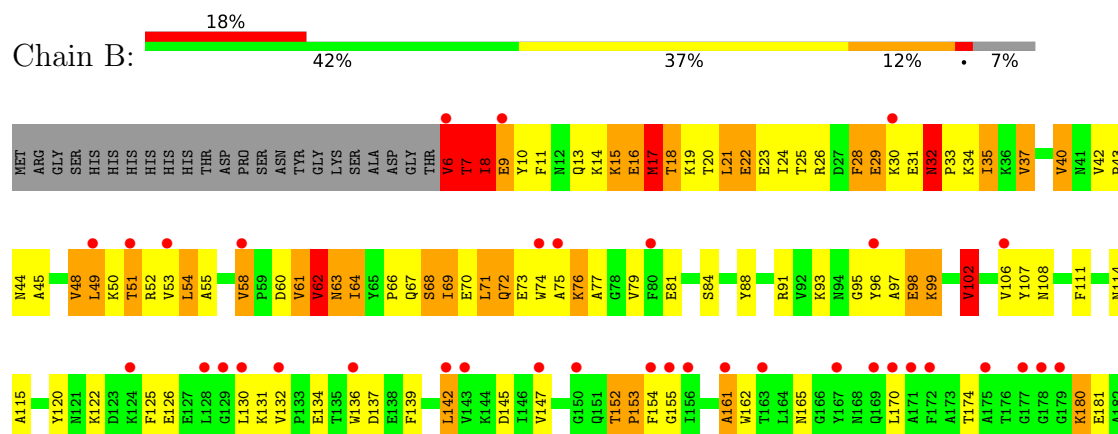
3 Residue-property plots

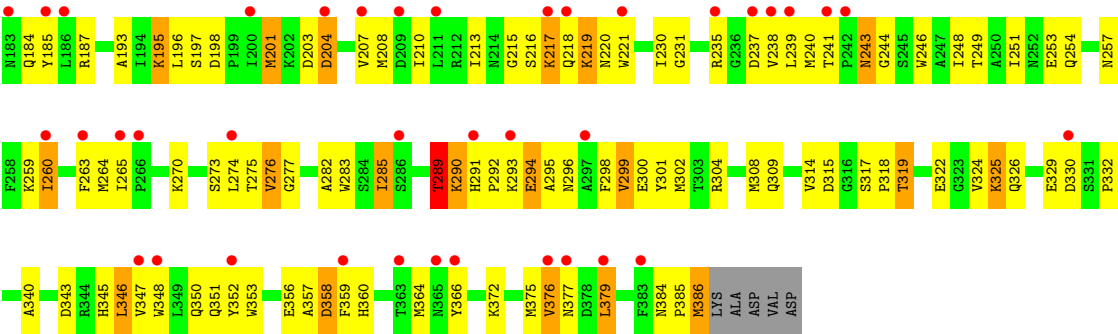
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Sugar ABC transporter, sugar-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	144.54Å 144.54Å 224.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.51 – 2.90 29.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.51-2.90) 99.0 (29.51-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.50 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.248 , 0.290 (Not available) , 0.285	Depositor DCC
R_{free} test set	1568 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	73.0	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 91.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6045	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: CL

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	1.44	19/3088 (0.6%)	1.57	45/4168 (1.1%)
1	B	1.14	17/3072 (0.6%)	1.51	64/4147 (1.5%)
All	All	1.30	36/6160 (0.6%)	1.54	109/8315 (1.3%)

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	1	1
1	B	0	4
All	All	1	5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	ILE	CA-CB	-9.96	1.42	1.54
1	A	36	LYS	CA-CB	-9.56	1.38	1.53
1	A	205	ILE	CA-CB	-8.26	1.44	1.54
1	B	377	ASN	CA-CB	-7.83	1.40	1.53
1	A	376	VAL	CA-CB	-7.70	1.45	1.54
1	A	94	ASN	CA-C	-7.61	1.46	1.53
1	B	358	ASP	CA-CB	-7.43	1.41	1.53
1	B	299	VAL	CA-CB	-6.64	1.47	1.54
1	A	75	ALA	CA-CB	-6.39	1.43	1.53
1	A	140	GLU	N-CA	-6.39	1.38	1.46
1	B	63	ASN	C-O	-6.32	1.16	1.24
1	A	115	ALA	C-O	6.28	1.31	1.23
1	B	139	PHE	CA-CB	6.23	1.63	1.53
1	A	324	VAL	CA-CB	-6.17	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	THR	C-O	-6.13	1.16	1.24
1	A	272	GLN	N-CA	-6.10	1.38	1.46
1	A	270	LYS	CA-CB	-6.09	1.43	1.53
1	B	142	LEU	CA-CB	-5.99	1.43	1.53
1	A	272	GLN	C-O	5.95	1.32	1.24
1	A	58	VAL	CA-C	5.88	1.57	1.53
1	B	197	SER	CA-CB	-5.80	1.43	1.53
1	A	320	ALA	CA-CB	-5.79	1.44	1.53
1	B	51	THR	C-O	5.76	1.31	1.24
1	B	291	HIS	CA-C	5.71	1.60	1.52
1	B	44	ASN	CA-C	5.65	1.60	1.53
1	B	204	ASP	CA-CB	-5.54	1.44	1.53
1	A	178	GLY	N-CA	5.53	1.51	1.45
1	A	269	GLU	CA-CB	-5.36	1.44	1.54
1	B	10	TYR	N-CA	5.34	1.52	1.46
1	B	185	TYR	CB-CG	-5.30	1.40	1.51
1	B	291	HIS	N-CA	5.27	1.53	1.46
1	A	153	PRO	N-CA	-5.26	1.40	1.47
1	A	368	LEU	N-CA	5.21	1.52	1.46
1	B	81	GLU	CD-OE2	5.20	1.35	1.25
1	B	45	ALA	N-CA	5.08	1.52	1.46
1	A	156	ILE	C-O	-5.03	1.18	1.24

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	PRO	CB-CA-C	-12.36	94.78	111.21
1	B	210	ILE	N-CA-CB	12.29	124.93	110.55
1	B	161	ALA	N-CA-C	11.49	130.32	111.37
1	B	215	GLY	N-CA-C	10.81	130.87	115.30
1	B	185	TYR	CB-CG-CD1	-10.71	104.74	120.80
1	B	185	TYR	CB-CG-CD2	10.65	136.78	120.80
1	B	216	SER	N-CA-C	10.59	122.82	111.28
1	A	31	GLU	N-CA-C	10.55	126.50	112.88
1	A	123	ASP	N-CA-C	-10.32	100.03	111.07
1	A	58	VAL	N-CA-C	9.98	117.21	108.63
1	B	359	PHE	CA-CB-CG	-9.38	104.42	113.80
1	A	19	LYS	CB-CA-C	9.30	125.37	110.95
1	A	31	GLU	N-CA-CB	-9.10	96.63	110.73
1	B	153	PRO	N-CA-C	8.98	126.31	113.47
1	B	28	PHE	CB-CA-C	-8.86	91.63	110.32
1	B	28	PHE	N-CA-C	8.82	123.14	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	ASP	N-CA-CB	8.64	122.82	109.94
1	B	45	ALA	N-CA-C	8.60	121.59	111.71
1	B	76	LYS	N-CA-C	-8.45	102.08	112.38
1	B	68	SER	N-CA-C	8.31	123.25	109.46
1	A	147	VAL	N-CA-C	-8.15	100.90	111.09
1	B	210	ILE	CB-CA-C	-7.97	101.77	111.97
1	B	68	SER	CB-CA-C	-7.97	96.73	109.80
1	B	29	GLU	N-CA-C	-7.87	101.52	112.45
1	A	290	LYS	CB-CA-C	7.83	125.34	109.76
1	A	65	TYR	CA-C-N	7.82	127.48	119.82
1	A	65	TYR	C-N-CA	7.82	127.48	119.82
1	B	62	VAL	N-CA-C	7.75	120.26	107.24
1	A	6	VAL	N-CA-C	7.47	118.20	110.05
1	B	8	ILE	N-CA-C	7.42	119.52	108.46
1	A	272	GLN	CA-C-O	7.40	127.40	119.34
1	A	219	LYS	CB-CA-C	-7.39	99.44	109.71
1	B	9	GLU	N-CA-C	7.32	120.85	109.07
1	B	58	VAL	CA-C-N	-7.31	112.47	119.85
1	B	58	VAL	C-N-CA	-7.31	112.47	119.85
1	B	153	PRO	CB-CA-C	-7.28	101.48	113.06
1	B	294	GLU	N-CA-C	7.25	123.25	113.97
1	B	7	THR	N-CA-C	7.24	120.79	110.14
1	A	283	TRP	N-CA-C	7.04	120.88	109.40
1	B	193	ALA	N-CA-C	7.03	122.15	113.50
1	B	170	LEU	CB-CA-C	-7.00	98.33	110.72
1	A	6	VAL	CB-CA-C	-6.89	104.01	111.59
1	B	75	ALA	CB-CA-C	-6.80	97.64	109.07
1	B	61	VAL	CA-C-N	-6.70	113.86	123.11
1	B	61	VAL	C-N-CA	-6.70	113.86	123.11
1	B	203	ASP	N-CA-CB	-6.65	100.28	110.13
1	A	272	GLN	CB-CA-C	6.62	121.57	110.44
1	A	330	ASP	N-CA-C	6.62	120.76	111.30
1	A	257	ASN	N-CA-C	6.57	120.76	113.21
1	A	344	ARG	N-CA-C	-6.50	104.92	112.92
1	B	17	MSE	N-CA-C	6.38	121.11	112.88
1	A	241	THR	CA-C-N	6.36	126.31	119.76
1	A	241	THR	C-N-CA	6.36	126.31	119.76
1	A	96	TYR	N-CA-C	6.36	118.74	111.11
1	B	161	ALA	CB-CA-C	-6.35	100.19	110.74
1	A	214	ASN	CB-CA-C	6.34	120.50	109.65
1	B	152	THR	CA-C-N	6.31	125.53	118.97
1	B	152	THR	C-N-CA	6.31	125.53	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	THR	N-CA-CB	6.26	119.53	110.20
1	B	18	THR	N-CA-C	6.24	124.09	110.80
1	B	291	HIS	N-CA-C	6.20	123.51	109.81
1	A	95	GLY	N-CA-C	-6.20	98.49	113.18
1	A	352	TYR	N-CA-C	-6.16	103.93	112.30
1	A	369	THR	N-CA-C	6.09	120.99	113.50
1	B	22	GLU	CA-C-N	-6.06	110.53	121.14
1	B	22	GLU	C-N-CA	-6.06	110.53	121.14
1	B	18	THR	N-CA-CB	-6.03	100.30	110.49
1	B	185	TYR	CA-CB-CG	6.03	124.75	113.90
1	B	243	ASN	N-CA-C	6.01	117.68	108.42
1	A	214	ASN	N-CA-C	-5.95	101.47	110.28
1	B	142	LEU	CB-CA-C	5.93	122.71	110.31
1	A	143	VAL	N-CA-C	-5.92	104.55	111.00
1	B	48	VAL	CB-CA-C	-5.86	104.37	112.04
1	A	329	GLU	CA-C-N	-5.82	113.42	123.25
1	A	329	GLU	C-N-CA	-5.82	113.42	123.25
1	B	19	LYS	CA-CB-CG	5.73	125.57	114.10
1	B	44	ASN	N-CA-C	5.70	119.29	111.54
1	B	358	ASP	CB-CA-C	5.70	121.60	110.67
1	B	317	SER	CA-C-N	5.68	125.61	119.76
1	B	317	SER	C-N-CA	5.68	125.61	119.76
1	A	288	THR	CB-CA-C	-5.66	102.33	111.28
1	B	43	PRO	N-CA-C	5.63	120.03	111.19
1	B	102	VAL	CB-CA-C	-5.58	104.28	111.53
1	B	19	LYS	CB-CA-C	-5.54	102.17	110.88
1	A	140	GLU	N-CA-C	-5.53	105.33	111.36
1	B	294	GLU	N-CA-CB	-5.51	103.01	110.67
1	A	79	VAL	N-CA-C	5.50	117.93	111.05
1	B	49	LEU	CB-CA-C	-5.50	102.02	110.81
1	A	386	MSE	N-CA-C	5.49	122.49	110.80
1	A	255	LYS	CA-CB-CG	5.49	125.07	114.10
1	B	139	PHE	CB-CA-C	-5.48	99.32	109.29
1	B	91	ARG	N-CA-C	-5.34	106.80	113.15
1	A	39	VAL	N-CA-C	5.31	114.95	106.88
1	B	77	ALA	N-CA-C	5.28	120.38	113.30
1	A	201	MSE	N-CA-C	-5.25	105.45	111.07
1	A	62	VAL	CB-CA-C	-5.21	103.07	110.83
1	B	276	VAL	N-CA-C	5.19	116.06	108.53
1	A	361	THR	CA-C-N	-5.15	112.86	120.28
1	A	361	THR	C-N-CA	-5.15	112.86	120.28
1	A	87	ASP	N-CA-C	-5.12	107.20	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	GLU	N-CA-C	5.10	117.97	111.69
1	B	44	ASN	N-CA-CB	5.10	119.44	111.84
1	B	207	VAL	N-CA-CB	5.07	117.44	110.54
1	A	133	PRO	CA-C-N	-5.06	114.54	122.79
1	A	133	PRO	C-N-CA	-5.06	114.54	122.79
1	B	210	ILE	CA-CB-CG1	-5.05	101.81	110.40
1	B	290	LYS	CB-CA-C	-5.05	100.58	109.62
1	A	274	LEU	CB-CA-C	-5.02	99.25	109.94
1	A	220	ASN	N-CA-CB	5.00	121.31	113.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	386	MSE	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	GLY	Peptide
1	B	154	PHE	Peptide
1	B	289	THR	Peptide
1	B	32	ASN	Peptide
1	B	6	VAL	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	3029	0	2968	175	0
1	B	3013	0	2948	194	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
All	All	6045	0	5916	360	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 33.

All (360) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ARG:HD2	1:B:187:ARG:O	1.43	1.15
1:A:387:LYS:HE2	1:A:387:LYS:O	1.44	1.14
1:A:6:VAL:HG11	1:A:291:HIS:CD2	1.81	1.14
1:B:62:VAL:HG23	1:B:64:ILE:HG22	1.28	1.14
1:B:32:ASN:O	1:B:35:ILE:HG13	1.48	1.11
1:A:6:VAL:CG1	1:A:291:HIS:CD2	2.36	1.09
1:B:289:THR:HG21	1:B:292:PRO:HB3	1.29	1.08
1:B:31:GLU:HG3	1:B:32:ASN:ND2	1.68	1.07
1:A:10:TYR:CE2	1:A:12:ASN:HB2	1.93	1.04
1:A:309:GLN:HE22	1:A:325:LYS:H	1.09	0.97
1:B:62:VAL:HG23	1:B:64:ILE:CG2	1.96	0.95
1:B:31:GLU:HG3	1:B:32:ASN:HD21	1.21	0.95
1:B:153:PRO:O	1:B:240:MSE:HE3	1.65	0.94
1:A:290:LYS:C	1:A:291:HIS:ND1	2.25	0.94
1:B:289:THR:CG2	1:B:292:PRO:HB3	1.98	0.93
1:B:13:GLN:H	1:B:63:ASN:ND2	1.66	0.93
1:A:124:LYS:HG3	1:A:239:LEU:CD2	1.99	0.92
1:B:264:MSE:HE3	1:B:275:THR:HG22	1.52	0.92
1:A:86:LYS:HE3	1:A:296:ASN:OD1	1.69	0.91
1:B:42:VAL:HG21	1:B:48:VAL:HG21	1.53	0.91
1:B:32:ASN:H	1:B:32:ASN:HD22	1.19	0.90
1:B:289:THR:HG21	1:B:292:PRO:CB	2.01	0.90
1:B:28:PHE:C	1:B:28:PHE:CD2	2.51	0.88
1:B:13:GLN:N	1:B:63:ASN:HD22	1.71	0.87
1:B:375:MSE:O	1:B:379:LEU:HG	1.75	0.86
1:B:208:MSE:HB3	1:B:366:TYR:HE2	1.39	0.85
1:B:79:VAL:HG12	1:B:79:VAL:O	1.75	0.85
1:A:70:GLU:OE2	1:A:70:GLU:N	2.09	0.84
1:A:291:HIS:HB3	1:A:294:GLU:CD	2.04	0.83
1:B:72:GLN:H	1:B:72:GLN:HE21	1.25	0.83
1:B:79:VAL:O	1:B:79:VAL:CG1	2.27	0.82
1:B:53:VAL:HG22	1:B:58:VAL:HG22	1.60	0.82
1:B:13:GLN:H	1:B:63:ASN:HD22	0.86	0.82
1:A:291:HIS:HB3	1:A:294:GLU:OE2	1.80	0.82
1:A:291:HIS:ND1	1:A:291:HIS:N	2.28	0.81
1:B:32:ASN:HD22	1:B:32:ASN:N	1.77	0.80
1:A:123:ASP:O	1:A:127:GLU:HG2	1.81	0.80
1:B:72:GLN:HE21	1:B:72:GLN:N	1.80	0.80
1:B:31:GLU:CG	1:B:32:ASN:HD21	1.94	0.79
1:B:32:ASN:ND2	1:B:32:ASN:N	2.30	0.79
1:B:289:THR:HG23	1:B:290:LYS:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:HG22	1:B:22:GLU:HG3	1.65	0.79
1:A:124:LYS:HG3	1:A:239:LEU:HD21	1.64	0.79
1:B:31:GLU:CG	1:B:32:ASN:ND2	2.46	0.78
1:B:208:MSE:HB3	1:B:366:TYR:CE2	2.19	0.78
1:A:192:ASN:H	1:A:384:ASN:HD21	1.30	0.78
1:A:124:LYS:HG3	1:A:239:LEU:HD22	1.64	0.78
1:B:376:VAL:HA	1:B:379:LEU:HD12	1.66	0.78
1:B:28:PHE:CD2	1:B:28:PHE:O	2.37	0.77
1:B:62:VAL:CG2	1:B:64:ILE:CG2	2.62	0.77
1:A:6:VAL:CG2	1:A:291:HIS:HD2	1.98	0.77
1:B:208:MSE:CB	1:B:366:TYR:HE2	1.97	0.77
1:B:187:ARG:O	1:B:187:ARG:CD	2.30	0.77
1:B:50:LYS:HA	1:B:74:TRP:CH2	2.19	0.77
1:B:24:ILE:HD13	1:B:302:MSE:HE1	1.67	0.76
1:B:50:LYS:HA	1:B:74:TRP:HH2	1.50	0.76
1:B:67:GLN:N	1:B:67:GLN:OE1	2.18	0.76
1:A:6:VAL:HG13	1:A:291:HIS:CD2	2.21	0.76
1:A:221:TRP:HZ3	1:A:364:MSE:HE1	1.48	0.76
1:B:17:MSE:HA	1:B:17:MSE:CE	2.16	0.75
1:A:387:LYS:O	1:A:387:LYS:CE	2.30	0.75
1:A:6:VAL:HG12	1:A:7:THR:N	2.01	0.74
1:B:17:MSE:SE	1:B:315:ASP:HB2	2.37	0.74
1:B:84:SER:OG	1:B:106:VAL:N	2.21	0.74
1:B:8:ILE:HG13	1:B:8:ILE:O	1.86	0.73
1:A:10:TYR:CZ	1:A:12:ASN:HB2	2.24	0.73
1:B:32:ASN:HB2	1:B:35:ILE:HD12	1.70	0.73
1:B:72:GLN:HB3	1:B:73:GLU:OE1	1.88	0.73
1:A:6:VAL:HG21	1:A:291:HIS:HD2	1.53	0.73
1:A:6:VAL:CG1	1:A:291:HIS:HD2	2.01	0.72
1:B:208:MSE:CB	1:B:366:TYR:CE2	2.72	0.72
1:B:32:ASN:HB2	1:B:35:ILE:CD1	2.19	0.72
1:B:11:PHE:CD1	1:B:40:VAL:HG12	2.26	0.71
1:B:32:ASN:HB3	1:B:35:ILE:HD11	1.73	0.70
1:B:134:GLU:HB3	1:B:270:LYS:HD2	1.74	0.70
1:B:32:ASN:CB	1:B:35:ILE:CD1	2.69	0.70
1:B:42:VAL:CG2	1:B:48:VAL:HG21	2.22	0.70
1:B:95:GLY:O	1:B:98:GLU:HB2	1.91	0.70
1:A:6:VAL:CG1	1:A:7:THR:N	2.54	0.70
1:A:154:PHE:O	1:A:238:VAL:HG11	1.92	0.69
1:B:17:MSE:HA	1:B:17:MSE:HE3	1.73	0.69
1:A:76:LYS:CG	1:A:76:LYS:O	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:TYR:CB	1:A:375:MSE:HE3	2.23	0.69
1:B:376:VAL:HA	1:B:379:LEU:CD1	2.21	0.69
1:A:34:LYS:O	1:A:35:ILE:HG13	1.93	0.69
1:B:24:ILE:HG21	1:B:302:MSE:HE1	1.75	0.69
1:B:69:ILE:O	1:B:73:GLU:HG2	1.93	0.69
1:B:51:THR:O	1:B:51:THR:OG1	2.11	0.68
1:B:289:THR:CG2	1:B:292:PRO:CB	2.67	0.68
1:B:162:TRP:H	1:B:162:TRP:CD1	2.10	0.67
1:A:225:GLY:O	1:A:228:ASP:HB2	1.94	0.67
1:B:309:GLN:HE22	1:B:325:LYS:H	1.42	0.67
1:A:152:THR:HB	1:A:238:VAL:HG12	1.76	0.67
1:B:318:PRO:HA	1:B:326:GLN:HE22	1.61	0.66
1:A:145:ASP:O	1:A:149:LYS:HG3	1.95	0.66
1:A:124:LYS:CG	1:A:239:LEU:HD22	2.26	0.66
1:B:111:PHE:CE1	1:B:302:MSE:HG3	2.30	0.66
1:A:108:ASN:HA	1:A:283:TRP:O	1.97	0.65
1:A:338:GLU:O	1:A:338:GLU:CG	2.45	0.65
1:A:161:ALA:HB1	1:A:360:HIS:O	1.97	0.65
1:A:12:ASN:ND2	1:A:41:ASN:OD1	2.30	0.65
1:A:152:THR:HB	1:A:238:VAL:CG1	2.26	0.65
1:B:69:ILE:HD12	1:B:69:ILE:H	1.60	0.64
1:A:77:ALA:O	1:B:15:LYS:HB3	1.98	0.64
1:A:350:GLN:HA	1:A:353:TRP:CG	2.32	0.64
1:B:294:GLU:N	1:B:294:GLU:OE1	2.31	0.64
1:B:62:VAL:CG2	1:B:64:ILE:HG22	2.14	0.64
1:A:276:VAL:HG22	1:A:277:GLY:N	2.13	0.63
1:A:56:GLY:HA3	1:B:40:VAL:HG22	1.80	0.63
1:A:283:TRP:HH2	1:A:302:MSE:HE2	1.64	0.63
1:B:153:PRO:O	1:B:240:MSE:HB2	1.98	0.63
1:B:219:LYS:O	1:B:220:ASN:HB2	1.98	0.62
1:A:366:TYR:HB3	1:A:375:MSE:HE3	1.81	0.62
1:A:6:VAL:HG11	1:A:291:HIS:CG	2.33	0.61
1:B:28:PHE:O	1:B:28:PHE:CG	2.50	0.61
1:B:155:GLY:HA3	1:B:238:VAL:HG21	1.82	0.61
1:A:34:LYS:C	1:A:35:ILE:HG13	2.25	0.61
1:A:179:GLY:H	1:A:346:LEU:HD22	1.65	0.61
1:A:387:LYS:HE2	1:A:387:LYS:C	2.24	0.61
1:A:384:ASN:N	1:A:385:PRO:HD2	2.16	0.61
1:B:50:LYS:HD3	1:B:70:GLU:HG2	1.83	0.60
1:A:366:TYR:HB3	1:A:375:MSE:CE	2.31	0.60
1:B:351:GLN:O	1:B:351:GLN:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:TYR:HB2	1:A:375:MSE:HE3	1.84	0.60
1:A:53:VAL:HA	1:A:58:VAL:HG22	1.85	0.59
1:B:289:THR:HG22	1:B:292:PRO:HG3	1.83	0.59
1:A:154:PHE:C	1:A:238:VAL:HG11	2.27	0.59
1:B:71:LEU:O	1:B:72:GLN:C	2.46	0.59
1:B:42:VAL:HG21	1:B:48:VAL:CG2	2.31	0.58
1:B:357:ALA:O	1:B:360:HIS:HB2	2.03	0.58
1:B:274:LEU:HB3	1:B:346:LEU:HD21	1.86	0.58
1:A:288:THR:CG2	1:B:22:GLU:HG3	2.31	0.58
1:A:291:HIS:CB	1:A:294:GLU:CD	2.75	0.58
1:B:102:VAL:CG2	1:B:107:TYR:HD2	2.17	0.58
1:A:89:LEU:HD11	1:A:106:VAL:HG11	1.85	0.57
1:A:190:GLN:OE1	1:A:190:GLN:HA	2.03	0.57
1:B:108:ASN:HD21	1:B:282:ALA:HB1	1.69	0.57
1:B:120:TYR:CD2	1:B:263:PHE:CD2	2.93	0.56
1:A:27:ASP:HA	1:A:30:LYS:HB2	1.88	0.56
1:A:221:TRP:CZ3	1:A:364:MSE:HE1	2.37	0.56
1:A:288:THR:CB	1:B:22:GLU:HG3	2.35	0.56
1:B:15:LYS:N	1:B:16:GLU:OE1	2.39	0.56
1:B:53:VAL:HG22	1:B:58:VAL:HG13	1.87	0.56
1:A:13:GLN:H	1:A:63:ASN:HD22	1.52	0.56
1:B:68:SER:O	1:B:68:SER:OG	2.23	0.56
1:A:6:VAL:HG11	1:A:291:HIS:HD2	1.58	0.56
1:A:76:LYS:O	1:A:76:LYS:HG3	2.05	0.56
1:B:24:ILE:HG21	1:B:302:MSE:CE	2.36	0.55
1:B:11:PHE:HD1	1:B:40:VAL:HG12	1.70	0.55
1:B:32:ASN:HB3	1:B:35:ILE:CD1	2.34	0.55
1:B:187:ARG:HD3	1:B:386:MSE:HE3	1.89	0.55
1:A:87:ASP:O	1:A:90:LYS:HB2	2.07	0.54
1:A:187:ARG:HD2	1:A:187:ARG:O	2.07	0.54
1:B:8:ILE:O	1:B:37:VAL:HA	2.07	0.54
1:B:28:PHE:O	1:B:32:ASN:ND2	2.40	0.54
1:A:294:GLU:O	1:A:297:ALA:HB3	2.07	0.54
1:A:380:ASN:O	1:A:384:ASN:HB2	2.08	0.54
1:B:230:ILE:HG23	1:B:251:ILE:HG13	1.90	0.53
1:B:289:THR:HG21	1:B:292:PRO:CA	2.39	0.53
1:B:187:ARG:HD2	1:B:187:ARG:C	2.29	0.53
1:B:201:MSE:O	1:B:201:MSE:SE	2.77	0.53
1:B:120:TYR:CD2	1:B:263:PHE:HD2	2.27	0.53
1:A:205:ILE:HD13	1:A:372:LYS:HG2	1.91	0.52
1:B:50:LYS:CA	1:B:74:TRP:HH2	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ILE:HG23	1:B:295:ALA:HB1	1.92	0.52
1:B:120:TYR:CD1	1:B:120:TYR:C	2.88	0.52
1:A:192:ASN:N	1:A:384:ASN:HD21	2.03	0.52
1:B:292:PRO:C	1:B:294:GLU:N	2.66	0.52
1:A:275:THR:HG23	1:A:345:HIS:HA	1.92	0.52
1:B:53:VAL:HG22	1:B:58:VAL:CG2	2.36	0.52
1:B:136:TRP:HE1	1:B:174:THR:HB	1.75	0.52
1:B:384:ASN:N	1:B:384:ASN:HD22	2.08	0.52
1:A:121:ASN:ND2	1:A:124:LYS:HG2	2.25	0.51
1:B:20:THR:O	1:B:21:LEU:C	2.53	0.51
1:A:6:VAL:CG1	1:A:7:THR:H	2.22	0.51
1:B:276:VAL:HG23	1:B:346:LEU:O	2.09	0.51
1:B:356:GLU:HG3	1:B:360:HIS:CE1	2.46	0.51
1:A:366:TYR:CB	1:A:375:MSE:CE	2.87	0.51
1:A:69:ILE:HD12	1:A:69:ILE:H	1.75	0.51
1:B:147:VAL:HG23	1:B:153:PRO:HG2	1.93	0.51
1:A:318:PRO:HA	1:A:326:GLN:HE22	1.76	0.51
1:B:69:ILE:O	1:B:72:GLN:HB2	2.11	0.51
1:B:239:LEU:O	1:B:240:MSE:HG3	2.11	0.51
1:A:121:ASN:HB3	1:A:124:LYS:HB2	1.93	0.50
1:A:161:ALA:HA	1:A:364:MSE:HG2	1.92	0.50
1:B:340:ALA:HA	1:B:345:HIS:ND1	2.27	0.50
1:A:169:GLN:HG2	1:A:349:LEU:HD12	1.94	0.50
1:A:53:VAL:HG11	1:A:74:TRP:CD2	2.46	0.50
1:B:136:TRP:HB2	1:B:137:ASP:OD1	2.12	0.50
1:B:289:THR:HG22	1:B:289:THR:O	2.11	0.50
1:B:345:HIS:O	1:B:345:HIS:CD2	2.65	0.50
1:A:384:ASN:C	1:A:386:MSE:N	2.69	0.49
1:A:6:VAL:CG2	1:A:291:HIS:CD2	2.88	0.49
1:B:221:TRP:HZ3	1:B:364:MSE:HE1	1.77	0.49
1:B:299:VAL:O	1:B:300:GLU:C	2.54	0.49
1:A:338:GLU:O	1:A:338:GLU:HG2	2.11	0.49
1:A:384:ASN:N	1:A:385:PRO:CD	2.76	0.49
1:B:162:TRP:O	1:B:165:ASN:HB2	2.12	0.49
1:B:308:MSE:HB3	1:B:324:VAL:HG21	1.95	0.49
1:A:25:THR:HG23	1:A:37:VAL:HB	1.95	0.48
1:A:276:VAL:HG22	1:A:277:GLY:H	1.76	0.48
1:A:283:TRP:HH2	1:A:302:MSE:CE	2.25	0.48
1:B:32:ASN:CB	1:B:35:ILE:HD12	2.35	0.48
1:A:111:PHE:HB2	1:A:281:LEU:O	2.13	0.48
1:B:181:GLU:OE1	1:B:181:GLU:N	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LYS:O	1:A:291:HIS:C	2.57	0.48
1:A:283:TRP:CH2	1:A:302:MSE:CE	2.97	0.48
1:A:179:GLY:H	1:A:346:LEU:CD2	2.24	0.48
1:A:179:GLY:O	1:A:180:LYS:C	2.57	0.48
1:A:82:ASP:OD2	1:A:105:LYS:HG2	2.13	0.48
1:A:232:ALA:HB1	1:A:237:ASP:HB2	1.96	0.48
1:A:244:GLY:HA3	1:A:246:TRP:CZ2	2.48	0.48
1:B:16:GLU:CD	1:B:16:GLU:H	2.21	0.48
1:A:123:ASP:CG	1:A:258:PHE:HB2	2.39	0.48
1:B:221:TRP:CZ3	1:B:364:MSE:HE1	2.48	0.48
1:B:345:HIS:CD2	1:B:345:HIS:C	2.92	0.48
1:A:384:ASN:C	1:A:386:MSE:H	2.21	0.48
1:A:210:ILE:HA	1:A:213:ILE:HD13	1.95	0.48
1:B:208:MSE:HB2	1:B:366:TYR:CE2	2.49	0.48
1:A:113:ALA:O	1:A:318:PRO:HG2	2.15	0.47
1:B:72:GLN:HE21	1:B:72:GLN:CA	2.22	0.47
1:B:69:ILE:H	1:B:69:ILE:CD1	2.16	0.47
1:B:17:MSE:O	1:B:21:LEU:HD22	2.14	0.47
1:A:308:MSE:O	1:A:309:GLN:C	2.57	0.47
1:B:48:VAL:O	1:B:52:ARG:HG2	2.15	0.47
1:A:124:LYS:CG	1:A:239:LEU:CD2	2.81	0.47
1:A:264:MSE:HE3	1:A:275:THR:HG22	1.97	0.47
1:A:312:TYR:C	1:A:314:VAL:H	2.23	0.47
1:B:8:ILE:HG13	1:B:37:VAL:HG13	1.97	0.47
1:A:152:THR:CB	1:A:238:VAL:HG12	2.44	0.47
1:A:309:GLN:NE2	1:A:325:LYS:H	1.93	0.47
1:B:120:TYR:HD2	1:B:263:PHE:CD2	2.32	0.47
1:B:260:ILE:HD13	1:B:332:PRO:HG3	1.97	0.47
1:B:248:ILE:HG23	1:B:249:THR:N	2.30	0.47
1:B:61:VAL:HG21	1:B:298:PHE:HD2	1.80	0.46
1:A:148:ALA:C	1:A:150:GLY:H	2.24	0.46
1:A:52:ARG:HB3	1:A:57:ASP:O	2.15	0.46
1:A:350:GLN:HA	1:A:353:TRP:CD2	2.51	0.46
1:A:295:ALA:O	1:A:296:ASN:C	2.56	0.46
1:B:11:PHE:HD1	1:B:40:VAL:CG1	2.28	0.46
1:B:31:GLU:O	1:B:33:PRO:HD3	2.15	0.46
1:B:204:ASP:O	1:B:208:MSE:HG2	2.16	0.46
1:A:212:ARG:HG3	1:A:212:ARG:HH11	1.81	0.46
1:B:6:VAL:CG2	1:B:7:THR:H	2.29	0.46
1:B:115:ALA:HA	1:B:276:VAL:O	2.16	0.46
1:B:29:GLU:C	1:B:31:GLU:N	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:GLY:O	1:B:347:VAL:HA	2.16	0.46
1:A:52:ARG:O	1:A:56:GLY:N	2.49	0.46
1:B:155:GLY:N	1:B:240:MSE:O	2.45	0.46
1:A:290:LYS:HB3	1:A:291:HIS:CE1	2.51	0.45
1:B:125:PHE:CD2	1:B:130:LEU:HB2	2.51	0.45
1:B:161:ALA:HB1	1:B:360:HIS:HB3	1.97	0.45
1:B:187:ARG:CD	1:B:187:ARG:C	2.88	0.45
1:A:76:LYS:O	1:A:76:LYS:HG2	2.15	0.45
1:A:253:GLU:C	1:A:255:LYS:N	2.75	0.45
1:A:221:TRP:CG	1:A:222:GLU:N	2.85	0.45
1:A:338:GLU:O	1:A:338:GLU:HG3	2.17	0.45
1:A:203:ASP:O	1:A:204:ASP:C	2.56	0.45
1:B:187:ARG:NE	1:B:352:TYR:O	2.50	0.45
1:B:218:GLN:O	1:B:221:TRP:HD1	2.00	0.45
1:A:350:GLN:C	1:A:353:TRP:H	2.25	0.45
1:B:88:TYR:OH	1:B:296:ASN:OD1	2.28	0.45
1:A:127:GLU:HG2	1:A:127:GLU:H	1.57	0.44
1:A:294:GLU:OE1	1:A:294:GLU:N	2.48	0.44
1:B:131:LYS:O	1:B:132:VAL:C	2.60	0.44
1:A:134:GLU:O	1:A:135:THR:HG23	2.16	0.44
1:A:196:LEU:HG	1:A:196:LEU:O	2.16	0.44
1:A:244:GLY:HA3	1:A:246:TRP:CE2	2.53	0.44
1:B:29:GLU:C	1:B:31:GLU:H	2.26	0.44
1:B:114:ASN:O	1:B:277:GLY:HA3	2.18	0.44
1:A:34:LYS:O	1:A:35:ILE:CG1	2.63	0.44
1:A:88:TYR:CD2	1:A:300:GLU:HB2	2.53	0.44
1:B:352:TYR:O	1:B:353:TRP:HD1	2.01	0.44
1:A:126:GLU:OE2	1:A:126:GLU:HA	2.17	0.44
1:A:253:GLU:C	1:A:255:LYS:H	2.25	0.44
1:B:73:GLU:O	1:B:76:LYS:N	2.51	0.44
1:B:195:LYS:O	1:B:198:ASP:CG	2.61	0.44
1:B:384:ASN:N	1:B:385:PRO:HD2	2.32	0.44
1:A:287:ALA:HB3	1:B:18:THR:HG21	2.00	0.44
1:A:350:GLN:C	1:A:352:TYR:N	2.72	0.44
1:A:157:ALA:N	1:A:229:VAL:HG21	2.33	0.43
1:A:354:THR:H	1:A:386:MSE:HE3	1.82	0.43
1:A:66:PRO:HB2	1:A:100:TYR:CD1	2.53	0.43
1:B:244:GLY:HA3	1:B:246:TRP:CH2	2.53	0.43
1:B:289:THR:HG23	1:B:290:LYS:C	2.42	0.43
1:A:60:ASP:OD1	1:A:289:THR:OG1	2.28	0.43
1:B:54:LEU:HD12	1:B:54:LEU:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:TYR:O	1:B:97:ALA:C	2.60	0.43
1:A:312:TYR:C	1:A:314:VAL:N	2.75	0.43
1:A:364:MSE:HE3	1:A:367:VAL:HB	2.00	0.43
1:B:348:TRP:HB3	1:B:350:GLN:OE1	2.19	0.43
1:A:42:VAL:O	1:A:45:ALA:HB2	2.19	0.43
1:A:203:ASP:O	1:A:206:LYS:HB3	2.17	0.43
1:A:11:PHE:CD2	1:A:49:LEU:HD13	2.54	0.43
1:A:65:TYR:O	1:A:68:SER:HB3	2.18	0.43
1:B:9:GLU:N	1:B:60:ASP:OD2	2.46	0.43
1:B:28:PHE:CE1	1:B:298:PHE:HA	2.54	0.43
1:A:99:LYS:HE2	1:A:343:ASP:OD1	2.18	0.43
1:A:121:ASN:CG	1:A:124:LYS:HG2	2.44	0.43
1:A:146:ILE:O	1:A:147:VAL:C	2.57	0.43
1:B:293:LYS:C	1:B:294:GLU:OE1	2.62	0.42
1:A:25:THR:CG2	1:A:37:VAL:HB	2.50	0.42
1:A:119:TYR:OH	1:A:245:SER:HA	2.20	0.42
1:A:328:GLY:O	1:A:330:ASP:N	2.52	0.42
1:A:362:LEU:HD12	1:A:362:LEU:C	2.44	0.42
1:B:301:TYR:O	1:B:304:ARG:HG3	2.19	0.42
1:A:57:ASP:O	1:A:57:ASP:OD1	2.37	0.42
1:A:56:GLY:HA3	1:B:40:VAL:CG2	2.47	0.42
1:B:66:PRO:HB3	1:B:108:ASN:ND2	2.34	0.42
1:A:28:PHE:HB2	1:A:301:TYR:CE2	2.54	0.42
1:A:276:VAL:CG2	1:A:277:GLY:N	2.81	0.42
1:B:180:LYS:HE2	1:B:184:GLN:OE1	2.20	0.42
1:B:111:PHE:HE2	1:B:283:TRP:HB2	1.85	0.42
1:B:217:LYS:O	1:B:218:GLN:C	2.62	0.42
1:B:244:GLY:HA3	1:B:246:TRP:CZ2	2.54	0.42
1:A:21:LEU:HA	1:A:21:LEU:HD12	1.58	0.42
1:A:87:ASP:OD2	1:A:87:ASP:N	2.52	0.42
1:A:260:ILE:HB	1:A:332:PRO:HB3	2.01	0.42
1:A:283:TRP:CZ3	1:A:302:MSE:HG2	2.55	0.42
1:A:319:THR:O	1:A:319:THR:HG23	2.19	0.42
1:A:262:THR:HB	1:A:336:MSE:HB2	2.02	0.42
1:A:117:GLY:CA	1:A:336:MSE:HE2	2.49	0.42
1:A:249:THR:O	1:A:253:GLU:HG3	2.20	0.42
1:B:17:MSE:HE1	1:B:314:VAL:HG11	2.01	0.42
1:B:26:ARG:O	1:B:29:GLU:HB2	2.20	0.42
1:A:82:ASP:OD1	1:A:82:ASP:C	2.63	0.41
1:B:20:THR:O	1:B:22:GLU:N	2.54	0.41
1:B:61:VAL:C	1:B:62:VAL:HG12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLY:C	1:A:118:ILE:HG12	2.41	0.41
1:B:308:MSE:HE2	1:B:319:THR:CB	2.50	0.41
1:A:288:THR:HA	1:B:22:GLU:HG3	2.03	0.41
1:B:49:LEU:HG	1:B:74:TRP:CZ3	2.55	0.41
1:B:76:LYS:HE2	1:B:76:LYS:HB2	1.89	0.41
1:A:181:GLU:O	1:A:182:ALA:C	2.61	0.41
1:A:247:ALA:O	1:A:248:ILE:C	2.62	0.41
1:B:102:VAL:HG23	1:B:107:TYR:HD2	1.86	0.41
1:B:231:GLY:HA2	1:B:254:GLN:OE1	2.20	0.41
1:A:65:TYR:HA	1:A:66:PRO:HD2	1.84	0.41
1:A:70:GLU:N	1:A:70:GLU:CD	2.78	0.41
1:B:99:LYS:H	1:B:99:LYS:HG2	1.55	0.41
1:A:173:ALA:CB	1:A:346:LEU:HD11	2.51	0.41
1:A:65:TYR:O	1:A:68:SER:CB	2.68	0.41
1:A:102:VAL:HG12	1:A:103:ASN:N	2.36	0.41
1:A:153:PRO:O	1:A:240:MSE:HB2	2.21	0.41
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.62	0.41
1:A:213:ILE:O	1:A:216:SER:OG	2.39	0.41
1:B:17:MSE:HE1	1:B:314:VAL:CG1	2.51	0.41
1:B:181:GLU:N	1:B:181:GLU:CD	2.79	0.41
1:B:347:VAL:HG12	1:B:348:TRP:O	2.20	0.41
1:A:83:LEU:O	1:A:89:LEU:HD13	2.20	0.41
1:B:50:LYS:HA	1:B:74:TRP:CZ2	2.56	0.41
1:B:53:VAL:CG2	1:B:58:VAL:HG13	2.51	0.41
1:A:288:THR:CA	1:B:22:GLU:HG3	2.51	0.40
1:B:122:LYS:HB2	1:B:259:LYS:O	2.21	0.40
1:B:147:VAL:CG2	1:B:153:PRO:HG2	2.52	0.40
1:B:347:VAL:HG12	1:B:348:TRP:N	2.35	0.40
1:A:152:THR:O	1:A:238:VAL:HG12	2.22	0.40
1:B:11:PHE:CD1	1:B:40:VAL:CG1	3.00	0.40
1:A:152:THR:HB	1:A:238:VAL:HG13	2.00	0.40
1:B:218:GLN:O	1:B:221:TRP:CD1	2.74	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	381/409 (93%)	339 (89%)	41 (11%)	1 (0%)	36	65
1	B	379/409 (93%)	325 (86%)	53 (14%)	1 (0%)	36	65
All	All	760/818 (93%)	664 (87%)	94 (12%)	2 (0%)	36	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	LYS
1	B	55	ALA

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	320/330 (97%)	271 (85%)	49 (15%)	3	9
1	B	318/330 (96%)	258 (81%)	60 (19%)	1	5
All	All	638/660 (97%)	529 (83%)	109 (17%)	2	7

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	12	ASN
1	A	16	GLU
1	A	19	LYS
1	A	20	THR
1	A	21	LEU
1	A	23	GLU
1	A	26	ARG
1	A	30	LYS
1	A	31	GLU

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Mol	Chain	Res	Type
1	A	53	VAL
1	A	54	LEU
1	A	57	ASP
1	A	62	VAL
1	A	69	ILE
1	A	70	GLU
1	A	72	GLN
1	A	76	LYS
1	A	83	LEU
1	A	84	SER
1	A	87	ASP
1	A	98	GLU
1	A	118	ILE
1	A	124	LYS
1	A	126	GLU
1	A	127	GLU
1	A	131	LYS
1	A	134	GLU
1	A	147	VAL
1	A	149	LYS
1	A	151	GLN
1	A	180	LYS
1	A	200	ILE
1	A	212	ARG
1	A	216	SER
1	A	217	LYS
1	A	222	GLU
1	A	227	THR
1	A	238	VAL
1	A	257	ASN
1	A	262	THR
1	A	290	LYS
1	A	291	HIS
1	A	329	GLU
1	A	330	ASP
1	A	360	HIS
1	A	361	THR
1	A	384	ASN
1	A	387	LYS
1	B	6	VAL
1	B	7	THR
1	B	8	ILE

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Mol	Chain	Res	Type
1	B	14	LYS
1	B	15	LYS
1	B	16	GLU
1	B	17	MSE
1	B	21	LEU
1	B	23	GLU
1	B	25	THR
1	B	30	LYS
1	B	32	ASN
1	B	34	LYS
1	B	35	ILE
1	B	37	VAL
1	B	40	VAL
1	B	54	LEU
1	B	62	VAL
1	B	64	ILE
1	B	69	ILE
1	B	71	LEU
1	B	72	GLN
1	B	93	LYS
1	B	98	GLU
1	B	99	LYS
1	B	102	VAL
1	B	126	GLU
1	B	142	LEU
1	B	145	ASP
1	B	152	THR
1	B	180	LYS
1	B	195	LYS
1	B	196	LEU
1	B	201	MSE
1	B	213	ILE
1	B	217	LYS
1	B	219	LYS
1	B	235	ARG
1	B	237	ASP
1	B	241	THR
1	B	243	ASN
1	B	253	GLU
1	B	257	ASN
1	B	260	ILE
1	B	265	ILE

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Mol	Chain	Res	Type
1	B	273	SER
1	B	285	ILE
1	B	289	THR
1	B	319	THR
1	B	322	GLU
1	B	325	LYS
1	B	329	GLU
1	B	330	ASP
1	B	343	ASP
1	B	346	LEU
1	B	358	ASP
1	B	372	LYS
1	B	376	VAL
1	B	379	LEU
1	B	386	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	63	ASN
1	A	151	GLN
1	A	184	GLN
1	A	257	ASN
1	A	291	HIS
1	A	296	ASN
1	A	309	GLN
1	A	326	GLN
1	A	384	ASN
1	B	32	ASN
1	B	63	ASN
1	B	72	GLN
1	B	103	ASN
1	B	108	ASN
1	B	220	ASN
1	B	309	GLN
1	B	326	GLN
1	B	380	ASN
1	B	384	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

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	372/409 (90%)	-0.05	7 (1%) 66 58	20, 65, 106, 160	19 (5%)
1	B	350/409 (85%)	1.15	74 (21%) 2 2	45, 108, 194, 234	51 (14%)
All	All	722/818 (88%)	0.53	81 (11%) 10 9	20, 85, 182, 234	70 (9%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	366	TYR	8.6
1	B	156	ILE	5.9
1	B	167	TYR	5.4
1	B	155	GLY	5.0
1	B	130	LEU	4.8
1	B	265	ILE	4.6
1	B	186	LEU	4.4
1	B	260	ILE	4.4
1	B	376	VAL	4.2
1	B	200	ILE	4.1
1	B	204	ASP	4.0
1	B	74	TRP	3.9
1	B	291	HIS	3.9
1	B	49	LEU	3.8
1	B	169	GLN	3.6
1	B	211	LEU	3.5
1	B	363	THR	3.4
1	A	387	LYS	3.3
1	B	235	ARG	3.3
1	B	379	LEU	3.2
1	A	285	ILE	3.2
1	B	239	LEU	3.1
1	B	365	ASN	3.1
1	B	51	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	359	PHE	3.1
1	A	33	PRO	3.1
1	A	238	VAL	3.0
1	B	383	PHE	3.0
1	B	75	ALA	3.0
1	B	286	SER	2.9
1	B	30	LYS	2.8
1	B	143	VAL	2.8
1	B	129	GLY	2.8
1	B	147	VAL	2.8
1	B	297	ALA	2.8
1	B	171	ALA	2.7
1	B	128	LEU	2.7
1	B	136	TRP	2.7
1	B	96	TYR	2.7
1	B	80	PHE	2.7
1	B	179	GLY	2.6
1	A	69	ILE	2.6
1	B	266	PRO	2.6
1	B	58	VAL	2.6
1	B	163	THR	2.6
1	B	6	VAL	2.5
1	B	170	LEU	2.5
1	B	347	VAL	2.5
1	B	9	GLU	2.4
1	B	348	TRP	2.4
1	B	221	TRP	2.4
1	A	290	LYS	2.4
1	B	207	VAL	2.4
1	B	241	THR	2.4
1	B	242	PRO	2.4
1	B	175	ALA	2.3
1	B	185	TYR	2.3
1	B	150	GLY	2.3
1	B	177	GLY	2.3
1	B	172	PHE	2.3
1	B	263	PHE	2.3
1	A	54	LEU	2.3
1	B	237	ASP	2.3
1	B	209	ASP	2.2
1	B	132	VAL	2.2
1	B	154	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	106	VAL	2.2
1	B	293	LYS	2.2
1	B	274	LEU	2.2
1	B	218	GLN	2.1
1	B	183	ASN	2.1
1	B	53	VAL	2.1
1	B	330	ASP	2.1
1	B	377	ASN	2.1
1	B	161	ALA	2.1
1	B	238	VAL	2.0
1	B	178	GLY	2.0
1	B	124	LYS	2.0
1	B	217	LYS	2.0
1	B	142	LEU	2.0
1	B	352	TYR	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](#)

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
2	CL	A	401	1/1	0.94	0.18	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.