



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 06:13 AM UTC

PDB ID : 1HQE / pdb_00001hqe
Title : HUMAN IMMUNODEFICIENCY VIRUS TYPE 1
Authors : Ding, J.; Hsiou, Y.; Arnold, E.
Deposited on : 2000-12-15
Resolution : 2.70 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
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

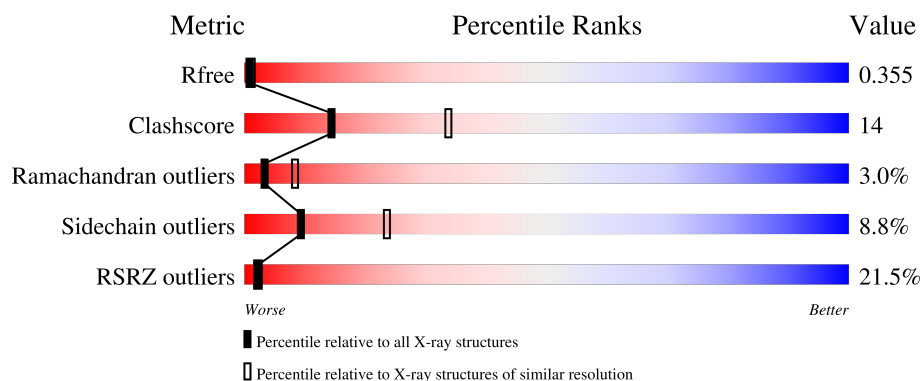
1 Overall quality at a glance

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	560	23% 64% 29% 6%
2	B	430	18% 53% 35% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7832 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 POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4349	2820	721	802	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	34	0	0
			3301	2142	547	607	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	103	ASN	LYS	engineered mutation	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

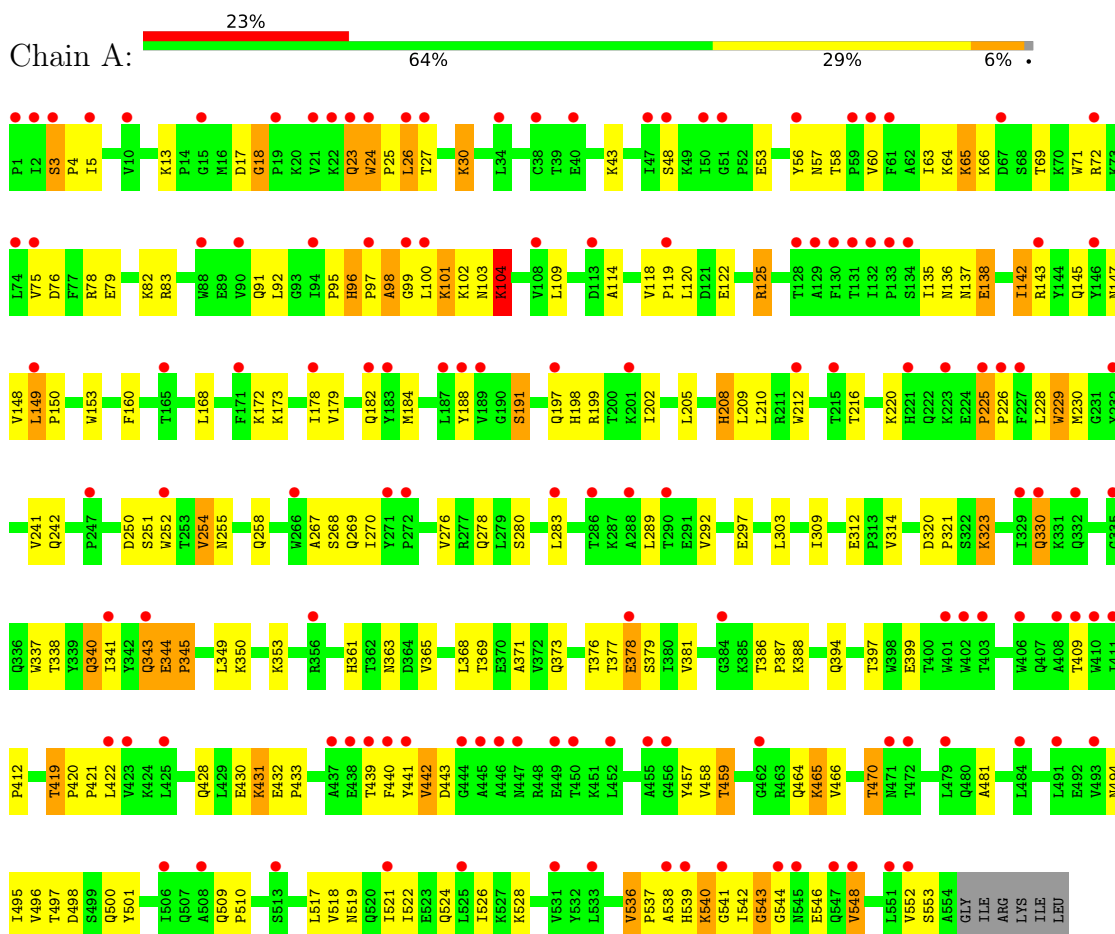
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total	O	0	0
			78	78		
3	B	104	Total	O	0	0
			104	104		

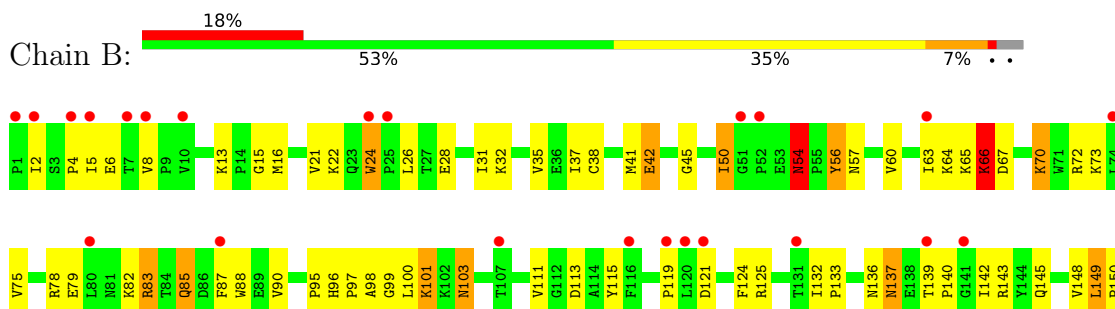
3 Residue-property plots

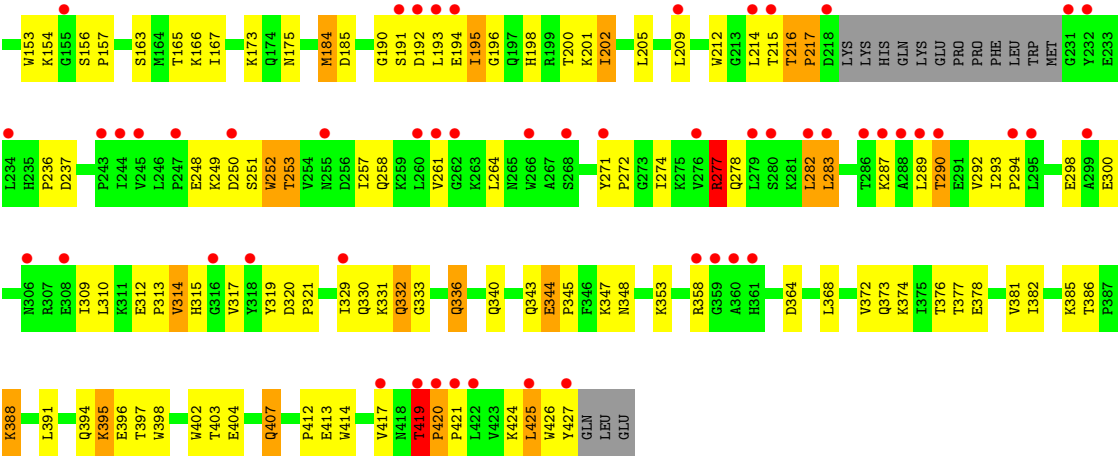
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 2: POL POLYPROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	236.10Å 70.40Å 93.40Å 90.00° 106.20° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 25.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	88.4 (25.00-2.70) 88.3 (25.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.68Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.250 , 0.331 0.306 , 0.355	Depositor DCC
R_{free} test set	1513 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7832	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.63	0/4467	1.22	48/6098 (0.8%)
2	B	0.66	0/3394	1.26	50/4626 (1.1%)
All	All	0.64	0/7861	1.24	98/10724 (0.9%)

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	2

There are no bond length outliers.

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	96	HIS	N-CA-C	11.16	123.30	109.57
2	B	420	PRO	N-CA-C	11.16	124.32	110.70
1	A	442	VAL	N-CA-C	10.94	121.97	110.05
1	A	420	PRO	N-CA-C	10.00	122.90	110.70
1	A	153	TRP	N-CA-C	9.59	122.71	110.24
1	A	344	GLU	CA-C-N	8.48	130.44	119.84
1	A	344	GLU	C-N-CA	8.48	130.44	119.84
1	A	258	GLN	N-CA-C	-8.41	102.07	111.07
2	B	63	ILE	N-CA-C	8.39	126.80	109.34
1	A	539	HIS	N-CA-C	8.35	121.82	112.97
2	B	195	ILE	N-CA-C	-8.16	101.97	113.07
2	B	414	TRP	N-CA-C	7.53	120.91	109.23
1	A	69	THR	N-CA-C	7.50	119.68	110.91
2	B	149	LEU	CA-C-N	7.50	128.09	119.99
2	B	149	LEU	C-N-CA	7.50	128.09	119.99
1	A	242	GLN	N-CA-C	-7.38	100.50	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	THR	N-CA-C	7.37	120.52	110.35
2	B	419	THR	CA-C-N	7.29	127.89	120.38
2	B	419	THR	C-N-CA	7.29	127.89	120.38
2	B	391	LEU	N-CA-C	7.26	120.08	109.04
2	B	419	THR	N-CA-C	7.25	125.82	109.81
1	A	138	GLU	N-CA-C	-7.19	104.13	113.12
1	A	538	ALA	N-CA-C	7.17	126.07	110.80
2	B	173	LYS	N-CA-C	-7.14	103.43	112.93
1	A	225	PRO	N-CA-C	7.08	119.34	110.70
1	A	388	LYS	N-CA-C	-7.06	98.54	109.76
1	A	13	LYS	N-CA-C	-6.98	101.28	109.93
1	A	71	TRP	N-CA-C	6.96	120.32	110.23
2	B	237	ASP	N-CA-C	-6.95	104.67	113.43
2	B	192	ASP	N-CA-C	6.93	121.19	112.87
2	B	425	LEU	N-CA-C	6.72	125.12	110.80
1	A	96	HIS	CA-C-N	6.72	127.26	119.47
1	A	96	HIS	C-N-CA	6.72	127.26	119.47
1	A	546	GLU	N-CA-C	-6.71	104.73	113.12
1	A	457	TYR	N-CA-C	6.69	120.72	110.36
1	A	3	SER	CA-C-N	6.69	127.22	119.47
1	A	3	SER	C-N-CA	6.69	127.22	119.47
2	B	277	ARG	N-CA-C	6.67	125.02	110.80
1	A	500	GLN	N-CA-C	-6.63	103.98	111.14
1	A	178	ILE	N-CA-C	6.53	117.98	108.58
2	B	216	THR	CA-C-N	6.48	127.94	119.84
2	B	216	THR	C-N-CA	6.48	127.94	119.84
2	B	317	VAL	N-CA-C	6.39	117.70	107.73
2	B	364	ASP	N-CA-C	6.33	117.98	111.14
2	B	424	LYS	N-CA-C	-6.27	102.59	111.56
1	A	191	SER	N-CA-C	6.23	117.69	108.60
2	B	388	LYS	N-CA-C	-6.20	99.76	109.25
1	A	18	GLY	N-CA-C	6.20	119.72	112.10
1	A	267	ALA	N-CA-C	6.06	118.67	111.33
1	A	297	GLU	N-CA-C	-6.05	104.80	111.82
2	B	417	VAL	N-CA-C	6.05	118.17	108.85
2	B	196	GLY	N-CA-C	-5.98	99.00	113.18
1	A	65	LYS	N-CA-C	5.91	118.28	108.99
2	B	65	LYS	N-CA-C	5.90	123.36	110.80
1	A	24	TRP	CA-C-N	5.83	127.12	119.84
1	A	24	TRP	C-N-CA	5.83	127.12	119.84
2	B	348	ASN	N-CA-C	5.80	118.68	110.50
2	B	377	THR	N-CA-C	-5.78	104.88	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	193	LEU	N-CA-C	5.77	117.17	108.46
1	A	343	GLN	N-CA-C	-5.75	104.25	112.13
1	A	419	THR	N-CA-C	-5.75	101.45	110.14
2	B	202	ILE	N-CA-C	-5.71	105.54	110.74
2	B	336	GLN	N-CA-C	5.71	118.26	110.55
2	B	344	GLU	N-CA-C	-5.68	100.31	109.40
1	A	184	MET	CB-CA-C	-5.67	110.02	116.54
1	A	149	LEU	CA-C-N	5.63	125.54	119.85
1	A	149	LEU	C-N-CA	5.63	125.54	119.85
2	B	252	TRP	N-CA-C	5.62	118.11	110.35
2	B	8	VAL	N-CA-C	5.56	113.42	108.63
1	A	98	ALA	N-CA-C	-5.54	106.60	113.19
1	A	119	PRO	N-CA-C	5.50	120.86	111.68
1	A	135	ILE	N-CA-C	-5.47	105.76	110.74
2	B	87	PHE	N-CA-C	5.45	117.18	108.41
2	B	56	TYR	N-CA-C	5.43	117.70	110.53
2	B	124	PHE	N-CA-C	5.43	118.12	111.82
2	B	358	ARG	N-CA-C	-5.43	105.78	112.90
2	B	13	LYS	CA-C-N	5.42	126.62	119.84
2	B	13	LYS	C-N-CA	5.42	126.62	119.84
2	B	64	LYS	N-CA-C	5.42	117.57	108.73
1	A	147	ASN	N-CA-C	-5.41	107.04	113.97
2	B	66	LYS	N-CA-C	5.41	122.32	110.80
2	B	16	MET	N-CA-C	5.37	118.23	110.28
2	B	300	GLU	N-CA-C	-5.34	106.27	112.89
2	B	282	LEU	N-CA-C	-5.34	106.77	113.28
1	A	278	GLN	N-CA-C	5.25	117.08	111.36
2	B	391	LEU	CA-C-N	5.23	126.38	119.84
2	B	391	LEU	C-N-CA	5.23	126.38	119.84
1	A	433	PRO	N-CA-C	5.22	119.44	111.34
1	A	432	GLU	CA-C-N	5.22	125.50	119.92
1	A	432	GLU	C-N-CA	5.22	125.50	119.92
1	A	30	LYS	N-CA-C	-5.21	105.68	111.36
1	A	182	GLN	N-CA-C	5.20	117.28	109.23
1	A	276	VAL	N-CA-C	-5.18	108.24	113.47
2	B	293	ILE	N-CA-C	5.13	112.94	107.76
2	B	165	THR	N-CA-C	-5.10	105.80	111.36
2	B	54	ASN	CA-C-N	5.07	124.68	119.56
2	B	54	ASN	C-N-CA	5.07	124.68	119.56
1	A	229	TRP	N-CA-C	5.02	116.80	108.02

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	TYR	Sidechain
1	A	501	TYR	Sidechain

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	4349	0	4251	106	2
2	B	3301	0	3228	111	1
3	A	78	0	0	7	0
3	B	104	0	0	8	1
All	All	7832	0	7479	213	2

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 14.

All (213) 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:465:LYS:HG2	3:A:620:HOH:O	0.93	1.10
2:B:57:ASN:HD22	2:B:143:ARG:HH21	1.05	0.97
1:A:142:ILE:H	1:A:142:ILE:HD13	1.27	0.96
2:B:332:GLN:HE22	2:B:427:TYR:H	1.12	0.96
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.54	0.87
2:B:314:VAL:HG12	2:B:315:HIS:H	1.39	0.87
2:B:57:ASN:HD22	2:B:143:ARG:NH2	1.80	0.79
2:B:253:THR:O	2:B:257:ILE:HD12	1.87	0.75
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.23	0.74
1:A:465:LYS:O	1:A:466:VAL:HG23	1.88	0.73
2:B:101:LYS:H	2:B:101:LYS:NZ	1.85	0.73
1:A:101:LYS:HD3	1:A:102:LYS:H	1.53	0.73
2:B:373:GLN:HE22	2:B:407:GLN:H	1.35	0.72
2:B:332:GLN:NE2	2:B:427:TYR:H	1.87	0.69
2:B:24:TRP:CD1	2:B:24:TRP:H	2.09	0.69
2:B:50:ILE:HD12	2:B:143:ARG:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.25	0.67
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.93	0.67
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.30	0.66
2:B:314:VAL:HG12	2:B:315:HIS:N	2.09	0.66
2:B:163:SER:O	2:B:167:ILE:HG13	1.95	0.66
1:A:544:GLY:O	1:A:548:VAL:HG23	1.96	0.65
2:B:70:LYS:HD3	2:B:70:LYS:H	1.60	0.65
2:B:101:LYS:H	2:B:101:LYS:HZ2	1.43	0.65
1:A:442:VAL:HG12	1:A:443:ASP:N	2.12	0.64
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.33	0.63
2:B:70:LYS:HD3	2:B:70:LYS:N	2.12	0.63
2:B:57:ASN:ND2	2:B:143:ARG:HH21	1.88	0.63
1:A:101:LYS:HD3	1:A:102:LYS:N	2.13	0.62
1:A:3:SER:OG	1:A:4:PRO:HD2	2.00	0.62
2:B:31:ILE:O	2:B:35:VAL:HG23	2.00	0.62
1:A:536:VAL:HG12	1:A:537:PRO:HD2	1.82	0.61
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.65	0.60
2:B:100:LEU:HG	2:B:381:VAL:HG13	1.84	0.59
2:B:332:GLN:HE22	2:B:427:TYR:N	1.93	0.58
1:A:199:ARG:HH22	1:A:220:LYS:HD2	1.68	0.58
1:A:464:GLN:O	1:A:465:LYS:HB2	2.02	0.58
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.04	0.58
2:B:344:GLU:O	2:B:347:LYS:HB2	2.03	0.58
1:A:78:ARG:O	1:A:82:LYS:HG3	2.03	0.57
1:A:26:LEU:H	1:A:26:LEU:HD12	1.69	0.57
1:A:343:GLN:HG2	1:A:349:LEU:HD11	1.86	0.57
2:B:157:PRO:HG3	2:B:184:MET:HA	1.87	0.57
2:B:277:ARG:HB3	2:B:278:GLN:HE21	1.70	0.57
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.19	0.56
1:A:378:GLU:O	1:A:378:GLU:HG2	2.04	0.56
1:A:540:LYS:O	1:A:542:ILE:N	2.35	0.56
2:B:373:GLN:NE2	2:B:407:GLN:H	2.03	0.56
1:A:254:VAL:HB	1:A:289:LEU:HA	1.86	0.56
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.46	0.56
2:B:24:TRP:CD1	2:B:24:TRP:N	2.73	0.56
1:A:517:LEU:O	1:A:521:ILE:HG13	2.06	0.56
2:B:42:GLU:HB3	3:B:472:HOH:O	2.06	0.56
1:A:518:VAL:O	1:A:522:ILE:HG12	2.07	0.55
2:B:309:ILE:O	2:B:309:ILE:HG22	2.07	0.55
1:A:199:ARG:HH12	1:A:220:LYS:HZ3	1.54	0.55
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PRO:C	1:A:99:GLY:H	2.14	0.54
2:B:137:ASN:HD22	2:B:137:ASN:N	2.05	0.54
2:B:312:GLU:OE2	2:B:313:PRO:HD2	2.08	0.54
1:A:341:ILE:HD12	1:A:350:LYS:HB3	1.90	0.54
2:B:38:CYS:O	2:B:42:GLU:HB2	2.08	0.53
1:A:95:PRO:HB3	2:B:136:ASN:O	2.08	0.53
1:A:376:THR:HG23	1:A:386:THR:HG22	1.91	0.53
1:A:142:ILE:HD13	1:A:142:ILE:N	2.11	0.53
2:B:50:ILE:HG12	2:B:145:GLN:HE21	1.73	0.53
1:A:268:SER:C	1:A:270:ILE:H	2.16	0.52
2:B:101:LYS:O	2:B:236:PRO:HB2	2.09	0.52
1:A:225:PRO:HG2	1:A:226:PRO:HD3	1.91	0.52
1:A:57:ASN:HD22	1:A:143:ARG:NH2	2.08	0.52
1:A:465:LYS:O	1:A:466:VAL:CG2	2.57	0.51
2:B:374:LYS:O	2:B:378:GLU:HB2	2.10	0.51
2:B:264:LEU:HD13	2:B:274:ILE:HD11	1.92	0.51
1:A:97:PRO:O	1:A:100:LEU:HB2	2.11	0.50
2:B:21:VAL:HG12	2:B:22:LYS:N	2.26	0.50
2:B:313:PRO:HG2	3:B:506:HOH:O	2.10	0.50
1:A:118:VAL:HG21	1:A:160:PHE:HD1	1.76	0.50
2:B:72:ARG:NH2	3:B:449:HOH:O	2.43	0.50
2:B:103:ASN:H	2:B:103:ASN:HD22	1.60	0.50
1:A:439:THR:HG22	1:A:494:ASN:HB2	1.93	0.50
2:B:149:LEU:HB3	2:B:156:SER:HB3	1.94	0.50
1:A:27:THR:OG1	1:A:30:LYS:HB2	2.13	0.49
2:B:314:VAL:CG1	2:B:315:HIS:H	2.19	0.49
1:A:419:THR:HG22	1:A:421:PRO:HD2	1.94	0.48
1:A:56:TYR:O	1:A:143:ARG:NH2	2.43	0.48
1:A:142:ILE:H	1:A:142:ILE:CD1	2.08	0.48
1:A:53:GLU:N	1:A:53:GLU:CD	2.71	0.48
1:A:309:ILE:O	1:A:312:GLU:HB3	2.12	0.48
1:A:498:ASP:HA	1:A:536:VAL:O	2.13	0.48
2:B:376:THR:CG2	2:B:386:THR:HG22	2.44	0.48
2:B:198:HIS:O	2:B:202:ILE:HG12	2.13	0.48
1:A:522:ILE:O	1:A:526:ILE:HG13	2.13	0.48
2:B:331:LYS:O	2:B:333:GLY:N	2.47	0.48
1:A:430:GLU:HA	1:A:431:LYS:HZ1	1.78	0.48
1:A:543:GLY:H	2:B:283:LEU:HD12	1.77	0.48
2:B:37:ILE:O	2:B:41:MET:HG3	2.14	0.48
2:B:54:ASN:HD21	2:B:56:TYR:HB2	1.79	0.48
2:B:163:SER:O	2:B:166:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:SER:HB3	2:B:294:PRO:HA	1.95	0.48
1:A:208:HIS:HE1	1:A:212:TRP:HE1	1.61	0.47
2:B:78:ARG:O	2:B:82:LYS:HG3	2.14	0.47
2:B:153:TRP:O	2:B:184:MET:SD	2.72	0.47
2:B:345:PRO:C	2:B:347:LYS:H	2.23	0.47
1:A:103:ASN:O	1:A:104:LYS:C	2.57	0.47
1:A:363:ASN:OD1	1:A:365:VAL:HG22	2.14	0.47
2:B:205:LEU:O	2:B:209:LEU:HG	2.15	0.47
1:A:442:VAL:CG1	1:A:443:ASP:N	2.76	0.47
1:A:109:LEU:HB3	1:A:216:THR:HG21	1.97	0.47
1:A:495:ILE:HG22	1:A:496:VAL:N	2.30	0.46
2:B:330:GLN:OE1	2:B:340:GLN:NE2	2.33	0.46
2:B:272:PRO:C	2:B:274:ILE:H	2.24	0.46
2:B:38:CYS:O	2:B:42:GLU:N	2.48	0.46
2:B:97:PRO:C	2:B:99:GLY:H	2.24	0.46
1:A:338:THR:HG22	1:A:353:LYS:HB3	1.97	0.46
1:A:97:PRO:C	1:A:99:GLY:N	2.72	0.45
1:A:350:LYS:HA	3:A:616:HOH:O	2.16	0.45
2:B:54:ASN:C	2:B:54:ASN:HD22	2.24	0.45
1:A:118:VAL:O	1:A:148:VAL:HG22	2.17	0.45
1:A:198:HIS:O	1:A:202:ILE:HG12	2.16	0.45
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.14	0.45
1:A:439:THR:HG21	2:B:289:LEU:H	1.82	0.45
1:A:509:GLN:N	1:A:510:PRO:HD3	2.31	0.45
2:B:388:LYS:NZ	2:B:413:GLU:HG3	2.31	0.45
1:A:377:THR:O	1:A:381:VAL:HG23	2.17	0.45
2:B:26:LEU:HD12	2:B:133:PRO:HG3	1.98	0.45
1:A:24:TRP:HA	1:A:25:PRO:HD2	1.77	0.45
2:B:66:LYS:CG	2:B:67:ASP:H	2.30	0.45
2:B:119:PRO:HA	2:B:148:VAL:HA	1.97	0.45
1:A:23:GLN:H	1:A:23:GLN:CD	2.24	0.45
1:A:191:SER:OG	1:A:198:HIS:CD2	2.70	0.45
2:B:184:MET:HB3	2:B:185:ASP:H	1.62	0.44
2:B:419:THR:HG22	2:B:421:PRO:HD2	1.98	0.44
1:A:241:VAL:HG23	1:A:314:VAL:O	2.17	0.44
2:B:85:GLN:C	2:B:85:GLN:HE21	2.25	0.44
2:B:139:THR:O	2:B:140:PRO:C	2.60	0.44
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.76	0.44
2:B:419:THR:HA	2:B:420:PRO:HD2	1.90	0.44
1:A:373:GLN:NE2	2:B:397:THR:HG23	2.32	0.44
2:B:216:THR:HA	2:B:217:PRO:HD2	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HG23	1:A:76:ASP:O	2.18	0.44
2:B:258:GLN:HG2	2:B:283:LEU:HD21	2.00	0.44
1:A:495:ILE:N	1:A:495:ILE:HD12	2.33	0.44
1:A:168:LEU:O	1:A:172:LYS:HG3	2.18	0.44
2:B:60:VAL:CG1	2:B:75:VAL:HG22	2.36	0.44
2:B:396:GLU:H	2:B:396:GLU:CD	2.25	0.44
1:A:344:GLU:HB3	1:A:345:PRO:HD2	2.00	0.43
2:B:385:LYS:HG2	2:B:386:THR:N	2.32	0.43
1:A:120:LEU:O	1:A:125:ARG:NE	2.51	0.43
1:A:337:TRP:O	1:A:353:LYS:HA	2.18	0.43
1:A:524:GLN:O	1:A:528:LYS:HG2	2.18	0.43
1:A:17:ASP:CG	1:A:18:GLY:H	2.26	0.43
2:B:154:LYS:O	2:B:157:PRO:HD2	2.19	0.43
1:A:519:ASN:HD22	1:A:519:ASN:H	1.65	0.43
2:B:394:GLN:O	2:B:395:LYS:C	2.62	0.43
1:A:101:LYS:CD	1:A:102:LYS:H	2.26	0.43
2:B:78:ARG:NH1	2:B:412:PRO:O	2.51	0.43
2:B:209:LEU:HB3	2:B:214:LEU:HB2	2.01	0.43
1:A:53:GLU:CD	1:A:53:GLU:H	2.27	0.43
1:A:441:TYR:HD1	1:A:441:TYR:N	2.15	0.43
1:A:441:TYR:N	1:A:441:TYR:CD1	2.86	0.43
1:A:63:ILE:HG22	1:A:64:LYS:N	2.33	0.43
2:B:319:TYR:O	2:B:321:PRO:HD3	2.19	0.43
1:A:118:VAL:O	1:A:148:VAL:CG2	2.66	0.43
2:B:298:GLU:H	2:B:298:GLU:HG2	1.60	0.43
2:B:5:ILE:HG22	2:B:5:ILE:O	2.19	0.42
1:A:205:LEU:O	1:A:209:LEU:HG	2.19	0.42
2:B:257:ILE:O	2:B:261:VAL:HG23	2.19	0.42
1:A:280:SER:HA	1:A:283:LEU:HD12	2.02	0.42
2:B:101:LYS:HE3	2:B:382:ILE:HA	2.02	0.42
2:B:190:GLY:HA2	3:B:450:HOH:O	2.18	0.42
1:A:229:TRP:O	1:A:230:MET:HB2	2.19	0.42
2:B:191:SER:OG	2:B:198:HIS:HD2	2.02	0.42
2:B:310:LEU:HD23	2:B:310:LEU:HA	1.85	0.42
2:B:330:GLN:NE2	2:B:340:GLN:OE1	2.46	0.42
2:B:32:LYS:HD2	3:B:480:HOH:O	2.19	0.42
1:A:228:LEU:HD23	3:A:570:HOH:O	2.20	0.42
2:B:329:ILE:HG22	2:B:330:GLN:N	2.34	0.42
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.82	0.41
1:A:122:GLU:HB2	3:A:604:HOH:O	2.19	0.41
1:A:252:TRP:O	1:A:292:VAL:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:GLY:HA2	3:B:484:HOH:O	2.20	0.41
2:B:79:GLU:HG3	2:B:83:ARG:HH11	1.84	0.41
2:B:66:LYS:HG2	2:B:67:ASP:N	2.36	0.41
2:B:121:ASP:O	2:B:125:ARG:HG3	2.20	0.41
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.77	0.41
2:B:320:ASP:H	2:B:343:GLN:HE22	1.67	0.41
2:B:137:ASN:N	2:B:137:ASN:ND2	2.67	0.41
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.84	0.41
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.20	0.41
1:A:440:PHE:CD1	1:A:440:PHE:N	2.87	0.41
2:B:97:PRO:C	2:B:99:GLY:N	2.79	0.41
2:B:336:GLN:HG2	2:B:353:LYS:HD3	2.03	0.41
1:A:320:ASP:OD2	1:A:323:LYS:HG3	2.21	0.41
1:A:368:LEU:O	1:A:371:ALA:HB3	2.21	0.41
2:B:332:GLN:NE2	2:B:426:TRP:HB2	2.36	0.41
1:A:5:ILE:H	1:A:5:ILE:HG13	1.58	0.41
1:A:495:ILE:CG2	1:A:496:VAL:N	2.84	0.41
2:B:250:ASP:N	3:B:491:HOH:O	2.42	0.41
1:A:136:ASN:C	1:A:138:GLU:H	2.29	0.41
2:B:28:GLU:O	2:B:32:LYS:HB2	2.21	0.41
2:B:368:LEU:O	2:B:372:VAL:HG23	2.21	0.41
1:A:199:ARG:HH12	1:A:220:LYS:NZ	2.18	0.40
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.20	0.40
2:B:184:MET:HE3	3:B:448:HOH:O	2.21	0.40
1:A:91:GLN:O	1:A:92:LEU:HB3	2.21	0.40
1:A:379:SER:OG	1:A:387:PRO:HD3	2.22	0.40
2:B:150:PRO:HB2	2:B:153:TRP:HB2	2.02	0.40
2:B:252:TRP:O	2:B:253:THR:O	2.39	0.40
2:B:398:TRP:O	2:B:402:TRP:HD1	2.04	0.40
1:A:548:VAL:HG11	3:A:566:HOH:O	2.20	0.40
2:B:66:LYS:CG	2:B:67:ASP:N	2.84	0.40
1:A:466:VAL:N	3:A:620:HOH:O	2.53	0.40
1:A:517:LEU:HG	3:A:617:HOH:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:CB	3:B:498:HOH:O[4_647]	1.80	0.40
1:A:251:SER:OG	2:B:15:GLY:O[4_647]	1.83	0.37

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	552/560 (99%)	488 (88%)	51 (9%)	13 (2%)	4	12
2	B	411/430 (96%)	345 (84%)	50 (12%)	16 (4%)	2	5
All	All	963/990 (97%)	833 (86%)	101 (10%)	29 (3%)	3	8

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	VAL
1	A	541	GLY
2	B	66	LYS
2	B	88	TRP
2	B	90	VAL
2	B	95	PRO
2	B	253	THR
2	B	277	ARG
2	B	332	GLN
1	A	345	PRO
2	B	2	ILE
2	B	425	LEU
1	A	104	LYS
1	A	125	ARG
1	A	137	ASN
1	A	412	PRO
1	A	470	THR
2	B	98	ALA
2	B	217	PRO
1	A	66	LYS
1	A	465	LYS
2	B	4	PRO
2	B	290	THR
2	B	292	VAL
2	B	395	LYS

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Mol	Chain	Res	Type
2	B	419	THR
1	A	269	GLN
1	A	543	GLY
1	A	552	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	452/500 (90%)	414 (92%)	38 (8%)	10	26
2	B	347/392 (88%)	315 (91%)	32 (9%)	8	22
All	All	799/892 (90%)	729 (91%)	70 (9%)	9	23

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	26	LEU
1	A	43	LYS
1	A	48	SER
1	A	60	VAL
1	A	65	LYS
1	A	72	ARG
1	A	75	VAL
1	A	101	LYS
1	A	104	LYS
1	A	142	ILE
1	A	145	GLN
1	A	173	LYS
1	A	179	VAL
1	A	197	GLN
1	A	208	HIS
1	A	210	LEU
1	A	254	VAL
1	A	255	ASN

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Mol	Chain	Res	Type
1	A	303	LEU
1	A	323	LYS
1	A	330	GLN
1	A	340	GLN
1	A	361	HIS
1	A	369	THR
1	A	378	GLU
1	A	399	GLU
1	A	409	THR
1	A	422	LEU
1	A	428	GLN
1	A	431	LYS
1	A	459	THR
1	A	470	THR
1	A	497	THR
1	A	536	VAL
1	A	540	LYS
1	A	548	VAL
1	A	553	SER
2	B	6	GLU
2	B	24	TRP
2	B	42	GLU
2	B	50	ILE
2	B	54	ASN
2	B	70	LYS
2	B	73	LYS
2	B	83	ARG
2	B	85	GLN
2	B	101	LYS
2	B	103	ASN
2	B	111	VAL
2	B	113	ASP
2	B	137	ASN
2	B	142	ILE
2	B	184	MET
2	B	194	GLU
2	B	195	ILE
2	B	200	THR
2	B	212	TRP
2	B	215	THR
2	B	248	GLU
2	B	249	LYS

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Mol	Chain	Res	Type
2	B	271	TYR
2	B	282	LEU
2	B	283	LEU
2	B	287	LYS
2	B	290	THR
2	B	314	VAL
2	B	404	GLU
2	B	407	GLN
2	B	419	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	145	GLN
1	A	197	GLN
1	A	198	HIS
1	A	222	GLN
1	A	306	ASN
1	A	330	GLN
1	A	340	GLN
1	A	373	GLN
1	A	428	GLN
1	A	471	ASN
1	A	519	ASN
1	A	524	GLN
1	A	545	ASN
2	B	54	ASN
2	B	57	ASN
2	B	85	GLN
2	B	103	ASN
2	B	137	ASN
2	B	145	GLN
2	B	147	ASN
2	B	198	HIS
2	B	255	ASN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	334	GLN
2	B	373	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](#)

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	554/560 (98%)	1.36	131 (23%) 2 1	22, 69, 100, 100	0
2	B	408/430 (94%)	1.11	76 (18%) 3 3	8, 58, 100, 100	0
All	All	962/990 (97%)	1.25	207 (21%) 2 2	8, 65, 100, 100	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	6.6
1	A	47	ILE	5.0
1	A	356	ARG	5.0
1	A	90	VAL	4.5
2	B	155	GLY	4.3
1	A	21	VAL	4.2
1	A	75	VAL	4.2
1	A	132	ILE	4.1
2	B	276	VAL	4.1
1	A	552	VAL	4.1
1	A	384	GLY	4.0
1	A	423	VAL	4.0
1	A	197	GLN	3.9
1	A	50	ILE	3.9
1	A	72	ARG	3.9
2	B	8	VAL	3.9
1	A	408	ALA	3.9
2	B	360	ALA	3.8
1	A	88	TRP	3.8
2	B	286	THR	3.8
1	A	38	CYS	3.7
1	A	60	VAL	3.7
1	A	439	THR	3.7
2	B	421	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	262	GLY	3.7
2	B	87	PHE	3.7
1	A	252	TRP	3.7
2	B	232	TYR	3.7
1	A	131	THR	3.6
1	A	171	PHE	3.6
2	B	283	LEU	3.5
2	B	420	PRO	3.5
1	A	134	SER	3.5
1	A	119	PRO	3.5
1	A	335	GLY	3.4
1	A	10	VAL	3.4
1	A	133	PRO	3.4
1	A	441	TYR	3.4
1	A	290	THR	3.4
1	A	409	THR	3.4
1	A	178	ILE	3.3
1	A	506	ILE	3.3
2	B	63	ILE	3.3
1	A	541	GLY	3.3
2	B	261	VAL	3.3
2	B	279	LEU	3.3
1	A	538	ALA	3.3
1	A	406	TRP	3.2
2	B	2	ILE	3.2
1	A	183	TYR	3.2
1	A	74	LEU	3.1
1	A	447	ASN	3.1
1	A	146	TYR	3.0
1	A	99	GLY	3.0
1	A	472	THR	3.0
1	A	513	SER	3.0
1	A	34	LEU	3.0
2	B	52	PRO	3.0
1	A	508	ALA	3.0
1	A	108	VAL	3.0
1	A	215	THR	3.0
1	A	130	PHE	3.0
1	A	479	LEU	2.9
1	A	59	PRO	2.9
1	A	143	ARG	2.9
1	A	329	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	7	THR	2.9
2	B	245	VAL	2.9
1	A	462	GLY	2.9
1	A	226	PRO	2.8
1	A	455	ALA	2.8
1	A	545	ASN	2.8
2	B	193	LEU	2.8
1	A	548	VAL	2.8
2	B	427	TYR	2.8
1	A	288	ALA	2.7
1	A	227	PHE	2.7
1	A	343	GLN	2.7
2	B	244	ILE	2.7
1	A	422	LEU	2.7
2	B	282	LEU	2.7
1	A	272	PRO	2.7
2	B	214	LEU	2.7
1	A	266	TRP	2.7
2	B	194	GLU	2.7
1	A	401	TRP	2.7
1	A	410	TRP	2.7
2	B	116	PHE	2.7
2	B	419	THR	2.7
2	B	294	PRO	2.7
2	B	5	ILE	2.6
2	B	289	LEU	2.6
1	A	456	GLY	2.6
1	A	48	SER	2.6
1	A	437	ALA	2.6
2	B	280	SER	2.6
1	A	97	PRO	2.6
2	B	107	THR	2.6
2	B	359	GLY	2.6
2	B	268	SER	2.6
1	A	67	ASP	2.6
1	A	2	ILE	2.6
2	B	80	LEU	2.5
2	B	218	ASP	2.5
1	A	22	LYS	2.5
2	B	1	PRO	2.5
1	A	445	ALA	2.5
1	A	450	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	212	TRP	2.5
2	B	141	GLY	2.5
2	B	191	SER	2.5
1	A	544	GLY	2.5
1	A	61	PHE	2.5
1	A	26	LEU	2.4
1	A	283	LEU	2.4
2	B	422	LEU	2.4
2	B	192	ASP	2.4
1	A	330	GLN	2.4
1	A	547	GLN	2.4
2	B	329	ILE	2.4
1	A	1	PRO	2.4
2	B	247	PRO	2.4
2	B	255	ASN	2.4
1	A	19	PRO	2.4
1	A	189	VAL	2.4
1	A	286	THR	2.4
1	A	221	HIS	2.4
2	B	288	ALA	2.4
1	A	187	LEU	2.3
1	A	271	TYR	2.3
1	A	533	LEU	2.3
1	A	27	THR	2.3
1	A	225	PRO	2.3
1	A	471	ASN	2.3
2	B	306	ASN	2.3
1	A	113	ASP	2.3
1	A	521	ILE	2.3
2	B	119	PRO	2.3
1	A	24	TRP	2.3
1	A	15	GLY	2.3
2	B	316	GLY	2.3
1	A	149	LEU	2.3
2	B	121	ASP	2.3
2	B	250	ASP	2.3
1	A	444	GLY	2.3
2	B	266	TRP	2.3
1	A	493	VAL	2.3
1	A	129	ALA	2.2
1	A	539	HIS	2.2
1	A	201	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	128	THR	2.2
2	B	131	THR	2.2
2	B	308	GLU	2.2
1	A	531	VAL	2.2
2	B	260	LEU	2.2
1	A	440	PHE	2.2
1	A	378	GLU	2.2
2	B	215	THR	2.2
1	A	182	GLN	2.2
2	B	24	TRP	2.2
2	B	361	HIS	2.2
2	B	139	THR	2.2
1	A	332	GLN	2.2
2	B	120	LEU	2.2
2	B	10	VAL	2.2
1	A	188	TYR	2.2
1	A	23	GLN	2.2
1	A	51	GLY	2.2
1	A	100	LEU	2.2
1	A	484	LEU	2.2
1	A	491	LEU	2.2
1	A	40	GLU	2.1
1	A	438	GLU	2.1
1	A	449	GLU	2.1
2	B	243	PRO	2.1
2	B	209	LEU	2.1
2	B	51	GLY	2.1
1	A	3	SER	2.1
2	B	417	VAL	2.1
1	A	402	TRP	2.1
2	B	4	PRO	2.1
2	B	25	PRO	2.1
2	B	425	LEU	2.1
1	A	5	ILE	2.1
1	A	411	ILE	2.1
1	A	425	LEU	2.1
2	B	234	LEU	2.1
2	B	271	TYR	2.1
2	B	318	TYR	2.1
1	A	94	ILE	2.1
1	A	452	LEU	2.1
1	A	525	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	551	LEU	2.1
1	A	165	THR	2.0
1	A	247	PRO	2.0
2	B	74	LEU	2.0
1	A	232	TYR	2.0
1	A	223	LYS	2.0
1	A	446	ALA	2.0
2	B	287	LYS	2.0
2	B	299	ALA	2.0
1	A	403	THR	2.0
2	B	290	THR	2.0
2	B	295	LEU	2.0
1	A	341	ILE	2.0
2	B	358	ARG	2.0
1	A	56	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.