



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:06 AM UTC

PDB ID : 4K0V / pdb_00004k0v
Title : Structural basis for angiopoietin-1 mediated signaling initiation
Authors : Yu, X.; Seegar, T.C.M.; Dalton, A.C.; Tzvetkova-Robev, D.; Goldgur, Y.;
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Deposited on : 2013-04-04
Resolution : 4.51 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

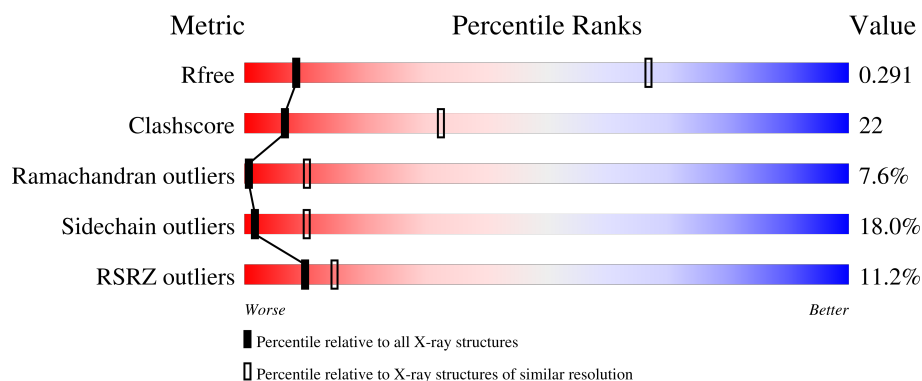
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.51 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	1131 (5.14-3.90)
Clashscore	190562	1005 (5.10-3.94)
Ramachandran outliers	187476	1061 (5.12-3.90)
Sidechain outliers	187428	1044 (5.12-3.90)
RSRZ outliers	180081	1126 (5.14-3.90)

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	529	
2	B	230	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5775 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 TEK tyrosine kinase variant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4021	2532	713	736	40			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	543	GLY	-	expression tag	UNP Q59HG2
A	544	SER	-	expression tag	UNP Q59HG2
A	545	ALA	-	expression tag	UNP Q59HG2
A	546	SER	-	expression tag	UNP Q59HG2
A	547	GLY	-	expression tag	UNP Q59HG2
A	548	LEU	-	expression tag	UNP Q59HG2
A	549	VAL	-	expression tag	UNP Q59HG2
A	550	PRO	-	expression tag	UNP Q59HG2
A	551	ARG	-	expression tag	UNP Q59HG2

- Molecule 2 is a protein called Angiopoietin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1754	1115	304	319	16			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ALA	-	expression tag	UNP Q15389
B	-3	GLU	-	expression tag	UNP Q15389
B	-2	LEU	-	expression tag	UNP Q15389
B	-1	ALA	-	expression tag	UNP Q15389
B	0	SER	-	expression tag	UNP Q15389
B	220	GLY	-	expression tag	UNP Q15389
B	221	SER	-	expression tag	UNP Q15389

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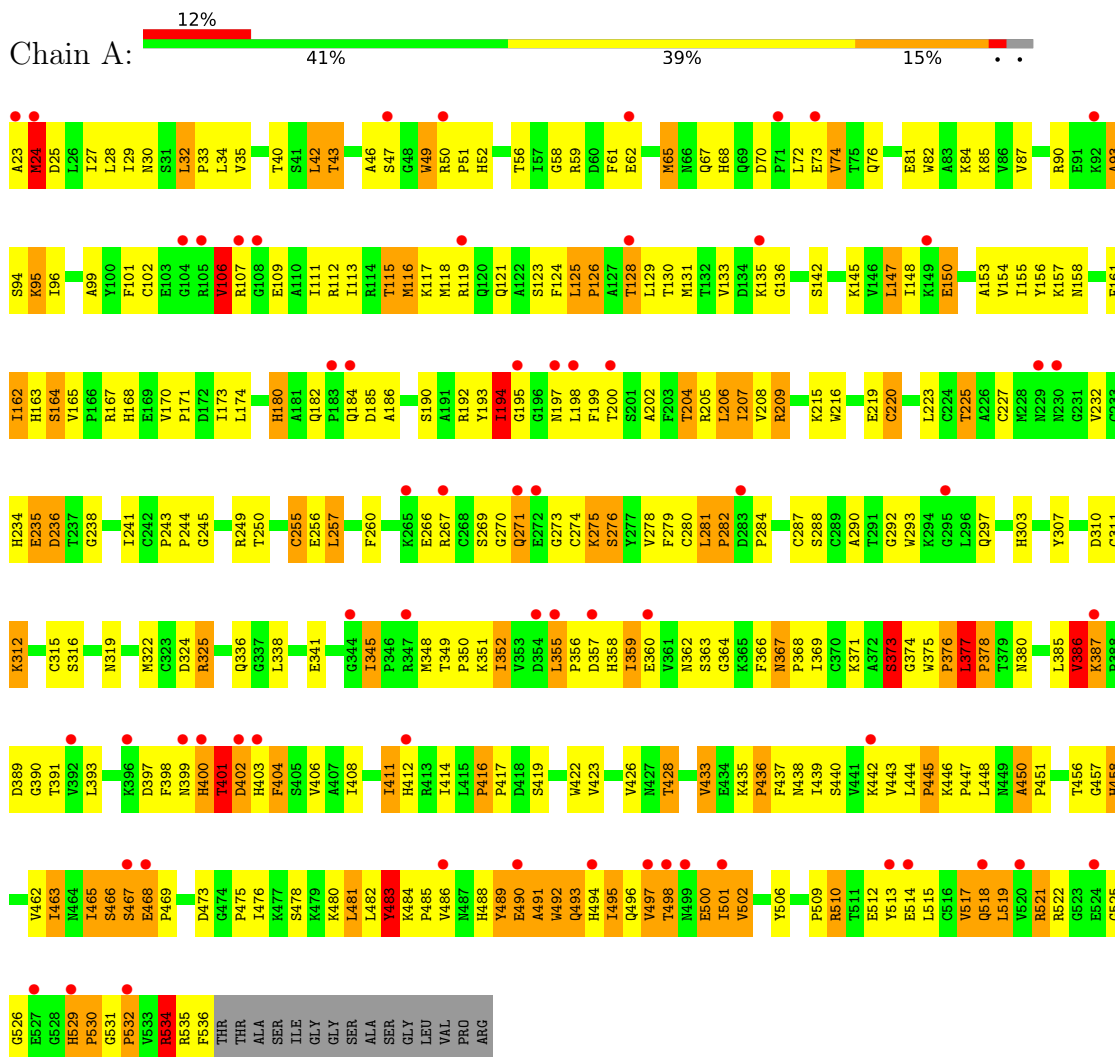
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Chain	Residue	Modelled	Actual	Comment	Reference
B	222	LEU	-	expression tag	UNP Q15389
B	223	VAL	-	expression tag	UNP Q15389
B	224	PRO	-	expression tag	UNP Q15389
B	225	ARG	-	expression tag	UNP Q15389

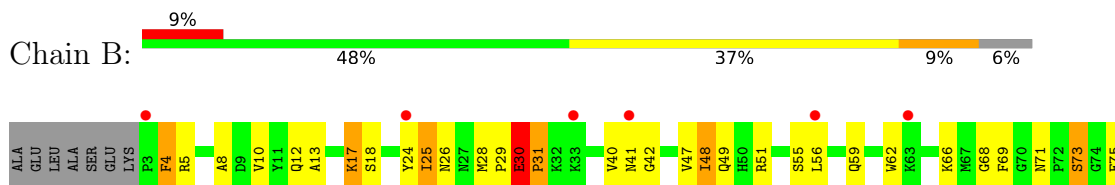
3 Residue-property plots

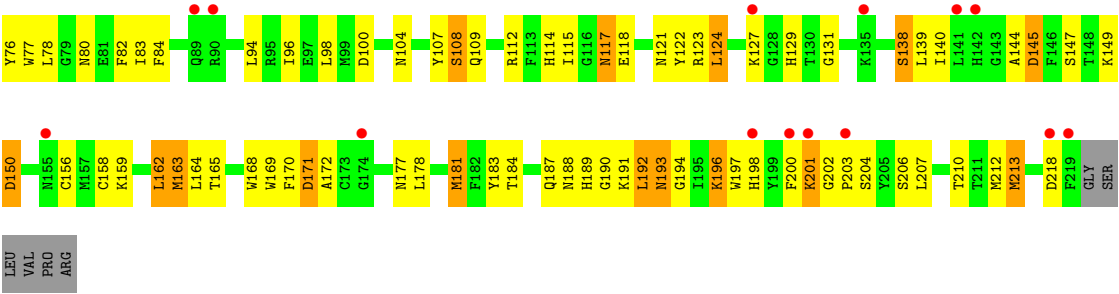
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: Angiopoietin-1





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	189.53Å 189.53Å 334.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.01 – 4.51 30.01 – 4.51	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.01-4.51) 91.4 (30.01-4.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.48 (at 4.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.248 , 0.288 0.249 , 0.291	Depositor DCC
R_{free} test set	542 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	141.8	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 190.8	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	0.87	EDS
Total number of atoms	5775	wwPDB-VP
Average B, all atoms (Å ²)	229.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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	0.74	1/4126 (0.0%)	1.21	34/5600 (0.6%)
2	B	0.58	0/1806	1.03	11/2433 (0.5%)
All	All	0.69	1/5932 (0.0%)	1.16	45/8033 (0.6%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	THR	CA-CB	6.68	1.62	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	ASN	CA-C-N	11.00	131.87	119.99
1	A	367	ASN	C-N-CA	11.00	131.87	119.99
1	A	500	GLU	N-CA-C	9.95	125.62	109.40
1	A	450	ALA	CA-C-N	-9.01	111.48	120.31
1	A	450	ALA	C-N-CA	-9.01	111.48	120.31
2	B	30	GLU	CA-C-N	8.59	130.57	119.84
2	B	30	GLU	C-N-CA	8.59	130.57	119.84
1	A	463	ILE	N-CA-C	8.47	119.53	108.35
2	B	76	TYR	N-CA-C	8.35	119.65	108.38
1	A	249	ARG	N-CA-C	-7.99	103.68	113.50
1	A	125	LEU	CA-C-N	7.06	128.66	119.84
1	A	125	LEU	C-N-CA	7.06	128.66	119.84
1	A	495	ILE	N-CA-C	6.59	118.07	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	198	HIS	N-CA-C	6.59	118.12	111.07
1	A	243	PRO	CA-C-N	6.44	127.89	119.84
1	A	243	PRO	C-N-CA	6.44	127.89	119.84
1	A	400	HIS	N-CA-C	-6.42	98.83	107.88
2	B	196	LYS	N-CA-C	6.16	119.59	109.85
1	A	377	LEU	CA-C-N	6.16	127.54	119.84
1	A	377	LEU	C-N-CA	6.16	127.54	119.84
1	A	483	TYR	N-CA-C	6.08	119.14	108.75
1	A	225	THR	N-CA-C	-6.07	101.20	110.30
1	A	501	ILE	N-CA-C	5.98	116.23	106.72
2	B	117	ASN	N-CA-C	5.93	117.74	109.31
1	A	198	LEU	N-CA-C	-5.92	106.10	113.15
1	A	303	HIS	CA-C-N	5.92	125.93	119.90
1	A	303	HIS	C-N-CA	5.92	125.93	119.90
1	A	386	VAL	N-CA-C	5.70	116.82	107.24
1	A	416	PRO	N-CA-C	5.67	117.61	110.70
1	A	194	ILE	N-CA-C	5.63	121.05	109.34
2	B	202	GLY	CA-C-N	5.60	125.70	119.32
2	B	202	GLY	C-N-CA	5.60	125.70	119.32
2	B	144	ALA	N-CA-C	-5.50	101.16	108.74
1	A	260	PHE	N-CA-C	5.42	117.03	108.96
1	A	521	ARG	N-CA-C	5.41	122.33	110.80
1	A	399	ASN	N-CA-C	-5.39	101.65	109.31
1	A	518	GLN	N-CA-C	5.27	117.26	108.99
1	A	534	ARG	N-CA-C	5.23	115.04	108.45
1	A	522	ARG	CB-CA-C	-5.20	110.60	116.63
2	B	131	GLY	N-CA-C	5.16	116.85	111.95
1	A	281	LEU	CA-C-N	5.10	126.22	119.84
1	A	281	LEU	C-N-CA	5.10	126.22	119.84
1	A	142	SER	N-CA-C	5.07	117.24	109.95
2	B	163	MET	N-CA-C	-5.06	106.45	113.18
1	A	164	SER	N-CA-C	5.02	115.16	108.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	467	SER	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	4021	0	3909	186	0
2	B	1754	0	1642	62	0
All	All	5775	0	5551	244	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 22.

All (244) 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:373:SER:OG	1:A:374:GLY:N	2.04	0.89
1:A:463:ILE:HD11	1:A:481:LEU:HD11	1.58	0.86
2:B:156:CYS:HB2	2:B:172:ALA:HA	1.57	0.86
1:A:450:ALA:HA	1:A:530:PRO:HB3	1.60	0.83
2:B:59:GLN:NE2	2:B:181:MET:SD	2.52	0.83
1:A:197:ASN:HB3	1:A:199:PHE:H	1.45	0.81
1:A:371:LYS:HG3	1:A:406:VAL:HG22	1.65	0.78
1:A:50:ARG:CZ	1:A:438:ASN:HD21	1.98	0.77
1:A:59:ARG:NH2	1:A:95:LYS:O	2.18	0.77
1:A:155:ILE:HG22	1:A:162:ILE:HD12	1.68	0.73
2:B:71:ASN:ND2	2:B:73:SER:OG	2.19	0.73
1:A:58:GLY:HA2	1:A:72:LEU:HD21	1.72	0.71
1:A:402:ASP:OD1	1:A:403:HIS:ND1	2.22	0.70
2:B:108:SER:HG	2:B:129:HIS:HE2	1.37	0.70
1:A:24:MET:SD	1:A:106:VAL:HG21	2.33	0.69
1:A:68:HIS:HB3	1:A:95:LYS:HD3	1.76	0.68
1:A:482:LEU:HD23	1:A:514:GLU:HB2	1.77	0.67
1:A:462:VAL:HG22	1:A:501:ILE:HG12	1.75	0.67
1:A:482:LEU:HA	1:A:491:ALA:HB1	1.77	0.66
1:A:445:PRO:HD3	1:A:519:LEU:HG	1.76	0.65
1:A:468:GLU:H	1:A:469:PRO:HD2	1.61	0.65
1:A:33:PRO:HA	1:A:117:LYS:HD2	1.79	0.65
1:A:130:THR:HG22	1:A:205:ARG:HB3	1.79	0.64
1:A:244:PRO:HD3	1:A:281:LEU:HD11	1.78	0.64
1:A:465:ILE:HB	1:A:498:THR:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:TYR:HB2	1:A:190:SER:HB2	1.80	0.64
1:A:126:PRO:HD3	1:A:202:ALA:HB1	1.80	0.64
1:A:359:ILE:HB	1:A:439:ILE:HA	1.79	0.64
1:A:150:GLU:HG3	1:A:167:ARG:HD3	1.80	0.63
2:B:147:SER:HB2	2:B:170:PHE:HD2	1.64	0.63
1:A:366:PHE:HB3	1:A:411:ILE:HD12	1.80	0.62
1:A:270:GLY:O	1:A:273:GLY:N	2.33	0.62
1:A:72:LEU:HD23	1:A:72:LEU:H	1.65	0.62
1:A:465:ILE:HG12	1:A:515:LEU:HD22	1.82	0.61
2:B:25:ILE:HB	2:B:28:MET:HG3	1.80	0.61
1:A:348:MET:HG3	1:A:375:TRP:H	1.64	0.61
2:B:140:ILE:HD13	2:B:171:ASP:HB2	1.83	0.61
1:A:52:HIS:HB3	1:A:82:TRP:CE2	2.35	0.60
1:A:513:TYR:O	1:A:531:GLY:HA2	2.01	0.60
2:B:40:VAL:O	2:B:42:GLY:N	2.35	0.60
2:B:178:LEU:HG	2:B:210:THR:HG21	1.84	0.60
1:A:59:ARG:HH12	1:A:70:ASP:HB3	1.66	0.60
1:A:234:HIS:CE1	1:A:236:ASP:HB2	2.37	0.59
1:A:32:LEU:O	1:A:117:LYS:NZ	2.36	0.58
1:A:241:ILE:HD13	1:A:282:PRO:HB2	1.84	0.58
2:B:78:LEU:HD23	2:B:83:ILE:HG13	1.86	0.58
1:A:136:GLY:HA2	1:A:180:HIS:HA	1.86	0.58
1:A:492:TRP:O	1:A:493:GLN:HB2	2.03	0.58
1:A:483:TYR:CD1	1:A:491:ALA:HA	2.39	0.57
1:A:67:GLN:NE2	1:A:99:ALA:H	2.02	0.57
1:A:59:ARG:NH1	1:A:70:ASP:HB3	2.20	0.57
1:A:348:MET:O	1:A:376:PRO:HD2	2.05	0.57
1:A:451:PRO:O	1:A:532:PRO:HG3	2.04	0.56
1:A:35:VAL:HG11	1:A:93:ALA:HB1	1.86	0.56
1:A:451:PRO:HD2	1:A:531:GLY:H	1.70	0.56
1:A:489:TYR:HD1	1:A:490:GLU:H	1.54	0.56
1:A:310:ASP:HB2	1:A:312:LYS:HG3	1.87	0.56
1:A:33:PRO:HG3	1:A:129:LEU:HD21	1.88	0.56
1:A:535:ARG:HG2	1:A:536:PHE:H	1.71	0.56
1:A:145:LYS:NZ	1:A:171:PRO:O	2.35	0.56
2:B:145:ASP:N	2:B:145:ASP:OD1	2.37	0.56
1:A:510:ARG:HA	1:A:534:ARG:O	2.06	0.55
2:B:190:GLY:HA2	2:B:204:SER:HB2	1.89	0.55
1:A:25:ASP:HB3	1:A:47:SER:HB2	1.89	0.55
1:A:355:LEU:HD12	1:A:356:PRO:CD	2.37	0.55
1:A:529:HIS:H	1:A:530:PRO:HD2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:VAL:HG11	1:A:284:PRO:O	2.09	0.53
1:A:350:PRO:HG3	1:A:428:THR:HG23	1.89	0.53
1:A:380:ASN:HB3	1:A:398:PHE:CD1	2.43	0.53
1:A:373:SER:HG	1:A:374:GLY:H	1.50	0.53
1:A:154:VAL:HG22	1:A:192:ARG:O	2.09	0.53
1:A:359:ILE:HG21	1:A:439:ILE:HG12	1.90	0.53
1:A:369:ILE:HG12	1:A:408:ILE:HG22	1.90	0.53
1:A:186:ALA:HB1	1:A:206:LEU:O	2.09	0.53
1:A:23:ALA:HB3	1:A:24:MET:SD	2.48	0.52
1:A:145:LYS:NZ	1:A:170:VAL:O	2.40	0.52
1:A:153:ALA:HB3	1:A:165:VAL:HB	1.92	0.52
2:B:29:PRO:O	2:B:30:GLU:HB2	2.09	0.52
1:A:375:TRP:C	1:A:377:LEU:N	2.67	0.51
2:B:24:TYR:CD2	2:B:31:PRO:HB3	2.45	0.51
2:B:62:TRP:O	2:B:66:LYS:N	2.43	0.51
1:A:128:THR:O	1:A:204:THR:OG1	2.25	0.51
1:A:307:TYR:HB2	1:A:324:ASP:O	2.10	0.51
1:A:397:ASP:HB3	1:A:408:ILE:HD11	1.93	0.51
1:A:400:HIS:ND1	1:A:401:THR:O	2.44	0.51
1:A:535:ARG:HG2	1:A:536:PHE:N	2.25	0.51
1:A:279:PHE:HE1	1:A:290:ALA:HB2	1.76	0.51
1:A:423:VAL:HG13	1:A:435:LYS:O	2.10	0.51
1:A:182:GLN:O	1:A:185:ASP:HB3	2.11	0.51
1:A:197:ASN:C	1:A:199:PHE:H	2.18	0.51
1:A:23:ALA:HB1	1:A:106:VAL:HG11	1.94	0.51
1:A:422:TRP:CD1	1:A:439:ILE:HD12	2.46	0.51
1:A:423:VAL:HG22	1:A:436:PRO:HB3	1.92	0.50
1:A:107:ARG:HD2	1:A:389:ASP:OD1	2.11	0.50
1:A:131:MET:HB3	1:A:206:LEU:HD23	1.94	0.50
2:B:66:LYS:NZ	2:B:118:GLU:OE1	2.23	0.50
1:A:375:TRP:C	1:A:377:LEU:H	2.20	0.50
1:A:483:TYR:HE2	1:A:502:VAL:HG11	1.76	0.50
1:A:50:ARG:NH2	1:A:438:ASN:HD21	2.10	0.50
1:A:359:ILE:HG22	1:A:360:GLU:N	2.27	0.50
2:B:4:PHE:CE1	2:B:10:VAL:HG22	2.48	0.49
1:A:401:THR:OG1	1:A:402:ASP:N	2.44	0.49
2:B:80:ASN:HB3	2:B:122:TYR:CD2	2.48	0.49
2:B:47:VAL:HG22	2:B:213:MET:HE2	1.93	0.49
1:A:197:ASN:HB3	1:A:200:THR:H	1.77	0.49
1:A:161:PHE:HE1	2:B:191:LYS:HD3	1.77	0.49
2:B:159:LYS:HB3	2:B:162:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:LYS:HD2	1:A:492:TRP:HZ3	1.78	0.49
2:B:8:ALA:O	2:B:12:GLN:HG2	2.13	0.49
1:A:43:THR:HG23	1:A:85:LYS:HB3	1.95	0.48
1:A:59:ARG:HB2	1:A:61:PHE:CE1	2.47	0.48
1:A:68:HIS:ND1	1:A:95:LYS:HD2	2.28	0.48
1:A:387:LYS:O	1:A:390:GLY:N	2.46	0.48
2:B:100:ASP:OD2	2:B:201:LYS:HE2	2.14	0.48
2:B:150:ASP:OD1	2:B:150:ASP:N	2.45	0.48
2:B:164:LEU:HB3	2:B:177:ASN:HD22	1.79	0.48
2:B:184:THR:OG1	2:B:187:GLN:OE1	2.30	0.48
1:A:192:ARG:NE	1:A:197:ASN:O	2.46	0.48
1:A:497:VAL:HG12	1:A:500:GLU:OE2	2.13	0.48
1:A:345:ILE:HD12	1:A:345:ILE:O	2.14	0.48
1:A:451:PRO:HB3	1:A:515:LEU:HD11	1.95	0.48
1:A:165:VAL:HG11	1:A:170:VAL:HA	1.95	0.47
1:A:68:HIS:HB3	1:A:95:LYS:CD	2.44	0.47
1:A:484:LYS:HE3	1:A:512:GLU:OE1	2.15	0.47
1:A:473:ASP:O	1:A:519:LEU:HD21	2.14	0.47
1:A:387:LYS:HG3	1:A:422:TRP:CZ3	2.49	0.47
2:B:149:LYS:O	2:B:162:LEU:HD21	2.14	0.47
1:A:125:LEU:HA	1:A:126:PRO:HD2	1.64	0.47
2:B:68:GLY:HA3	2:B:78:LEU:O	2.15	0.47
2:B:115:ILE:HD12	2:B:122:TYR:HB3	1.96	0.47
2:B:181:MET:HB2	2:B:193:ASN:O	2.15	0.47
1:A:46:ALA:HB3	1:A:82:TRP:HD1	1.80	0.47
1:A:209:ARG:CB	1:A:235:GLU:HG2	2.45	0.47
1:A:292:GLY:HA2	1:A:325:ARG:O	2.14	0.47
1:A:387:LYS:HD2	1:A:393:LEU:HD11	1.97	0.47
2:B:162:LEU:H	2:B:162:LEU:HG	1.45	0.47
1:A:76:GLN:HE21	1:A:82:TRP:HZ3	1.63	0.47
1:A:147:LEU:O	1:A:193:TYR:HE1	1.97	0.47
1:A:366:PHE:O	1:A:368:PRO:HD3	2.15	0.47
1:A:416:PRO:N	1:A:417:PRO:HD2	2.30	0.47
1:A:447:PRO:HB3	1:A:467:SER:OG	2.15	0.47
1:A:364:GLY:O	1:A:414:ILE:HG22	2.15	0.46
1:A:480:LYS:HD2	1:A:492:TRP:CZ3	2.50	0.46
1:A:155:ILE:CG2	1:A:162:ILE:HD12	2.44	0.46
1:A:274:CYS:C	1:A:276:SER:H	2.23	0.46
2:B:200:PHE:CE2	2:B:201:LYS:HG2	2.49	0.46
1:A:162:ILE:O	2:B:192:LEU:HD12	2.16	0.46
2:B:100:ASP:OD1	2:B:104:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:LEU:HD22	2:B:207:LEU:HD13	1.98	0.46
2:B:168:TRP:CG	2:B:169:TRP:H	2.34	0.46
2:B:183:TYR:CE2	2:B:191:LYS:HB3	2.51	0.46
1:A:153:ALA:O	1:A:164:SER:HB2	2.15	0.45
1:A:352:ILE:HD11	1:A:426:VAL:HG23	1.98	0.45
1:A:426:VAL:HB	1:A:433:VAL:HG23	1.99	0.45
2:B:48:ILE:HD11	2:B:212:MET:HE2	1.97	0.45
1:A:345:ILE:HD11	1:A:375:TRP:CZ2	2.51	0.45
2:B:187:GLN:O	2:B:189:HIS:N	2.50	0.45
1:A:312:LYS:HB3	1:A:312:LYS:HE2	1.73	0.45
1:A:115:THR:HG22	1:A:116:MET:H	1.82	0.45
2:B:192:LEU:C	2:B:194:GLY:H	2.25	0.45
1:A:34:LEU:HD23	1:A:118:MET:HG3	1.99	0.45
1:A:163:HIS:HB2	2:B:203:PRO:HB2	1.99	0.45
1:A:32:LEU:HD22	1:A:297:GLN:NE2	2.32	0.45
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.72	0.45
1:A:468:GLU:H	1:A:469:PRO:CD	2.29	0.45
1:A:197:ASN:HB3	1:A:199:PHE:N	2.24	0.44
2:B:84:PHE:CZ	2:B:117:ASN:HB3	2.52	0.44
1:A:466:SER:H	1:A:515:LEU:CD1	2.30	0.44
1:A:28:LEU:HD23	1:A:102:CYS:SG	2.58	0.44
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.70	0.44
1:A:377:LEU:HA	1:A:378:PRO:HD2	1.62	0.44
2:B:25:ILE:HD12	2:B:82:PHE:HD2	1.82	0.44
2:B:17:LYS:HG3	2:B:18:SER:N	2.33	0.44
2:B:68:GLY:HA2	2:B:77:TRP:HD1	1.83	0.44
1:A:275:LYS:HG3	1:A:293:TRP:CZ3	2.52	0.44
2:B:26:ASN:C	2:B:28:MET:H	2.25	0.44
2:B:96:ILE:HG12	2:B:212:MET:HG2	1.99	0.44
1:A:476:ILE:HG12	1:A:517:VAL:CG1	2.48	0.44
1:A:119:ARG:HE	1:A:200:THR:HA	1.82	0.44
1:A:366:PHE:C	1:A:368:PRO:HD3	2.42	0.44
1:A:67:GLN:HE22	1:A:99:ALA:H	1.62	0.43
1:A:157:LYS:HG2	1:A:158:ASN:N	2.32	0.43
1:A:448:LEU:CB	1:A:469:PRO:HB2	2.48	0.43
2:B:124:LEU:HB2	2:B:169:TRP:CD1	2.53	0.43
1:A:32:LEU:HA	1:A:32:LEU:HD23	1.67	0.43
1:A:131:MET:O	1:A:207:ILE:HG13	2.19	0.43
2:B:183:TYR:HB2	2:B:206:SER:CB	2.49	0.43
1:A:163:HIS:CG	1:A:164:SER:N	2.87	0.43
1:A:456:THR:HG22	1:A:457:GLY:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:O	1:A:208:VAL:HA	2.19	0.43
1:A:156:TYR:O	1:A:190:SER:N	2.47	0.43
1:A:245:GLY:O	1:A:255:CYS:HB2	2.19	0.43
1:A:76:GLN:NE2	1:A:82:TRP:HZ3	2.17	0.43
1:A:47:SER:OG	1:A:266:GLU:OE2	2.36	0.43
2:B:121:ASN:HB3	2:B:145:ASP:HB3	2.00	0.43
1:A:194:ILE:HG13	2:B:163:MET:HE1	2.00	0.42
2:B:25:ILE:HB	2:B:28:MET:CG	2.46	0.42
1:A:30:ASN:HA	1:A:42:LEU:HD12	2.01	0.42
1:A:90:ARG:HE	1:A:90:ARG:HB3	1.48	0.42
1:A:322:MET:HE2	1:A:322:MET:HB3	1.94	0.42
1:A:225:THR:HG22	1:A:250:THR:HG22	2.02	0.42
1:A:448:LEU:CD2	1:A:469:PRO:HB2	2.48	0.42
2:B:138:SER:HB2	2:B:197:TRP:CE2	2.53	0.42
2:B:25:ILE:HB	2:B:28:MET:HB2	2.01	0.42
1:A:442:LYS:HD2	1:A:442:LYS:HA	1.74	0.42
1:A:74:VAL:HG12	1:A:84:LYS:HB3	2.02	0.42
1:A:194:ILE:HG23	1:A:195:GLY:H	1.84	0.42
1:A:386:VAL:HG22	1:A:423:VAL:O	2.20	0.42
1:A:444:LEU:H	1:A:444:LEU:HG	1.65	0.42
1:A:52:HIS:HB3	1:A:82:TRP:CD2	2.55	0.42
1:A:450:ALA:O	1:A:466:SER:HB2	2.20	0.42
1:A:456:THR:HG22	1:A:457:GLY:H	1.85	0.42
1:A:216:TRP:CE2	1:A:238:GLY:HA3	2.55	0.42
1:A:65:MET:HG2	1:A:158:ASN:O	2.20	0.42
1:A:482:LEU:HD12	1:A:491:ALA:CB	2.50	0.42
2:B:56:LEU:HD21	2:B:69:PHE:CD1	2.55	0.42
1:A:33:PRO:HD2	1:A:297:GLN:NE2	2.35	0.41
1:A:40:THR:OG1	1:A:117:LYS:HE3	2.20	0.41
1:A:235:GLU:H	1:A:235:GLU:HG3	1.59	0.41
1:A:360:GLU:HA	1:A:440:SER:O	2.19	0.41
1:A:478:SER:HB3	1:A:518:GLN:OE1	2.18	0.41
1:A:197:ASN:CB	1:A:200:THR:H	2.33	0.41
1:A:50:ARG:NH1	1:A:438:ASN:HD21	2.17	0.41
1:A:215:LYS:HE3	1:A:220:CYS:O	2.19	0.41
1:A:422:TRP:HB2	1:A:437:PHE:CE1	2.55	0.41
1:A:445:PRO:HB2	1:A:517:VAL:HB	2.02	0.41
1:A:416:PRO:O	1:A:419:SER:OG	2.23	0.41
2:B:168:TRP:CD1	2:B:169:TRP:H	2.38	0.41
1:A:362:ASN:OD1	1:A:519:LEU:HD12	2.21	0.41
1:A:113:ILE:HD13	1:A:280:CYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:LYS:HD3	1:A:494:HIS:CE1	2.55	0.41
2:B:201:LYS:HD2	2:B:201:LYS:HA	1.79	0.41
2:B:112:ARG:HB2	2:B:127:LYS:HB3	2.02	0.41
1:A:33:PRO:HD3	1:A:278:VAL:HG21	2.03	0.41
2:B:51:ARG:HA	2:B:75:GLU:HG2	2.01	0.41
1:A:135:LYS:HE3	1:A:182:GLN:OE1	2.20	0.41
1:A:162:ILE:HB	1:A:163:HIS:H	1.41	0.41
2:B:94:LEU:HD12	2:B:213:MET:O	2.21	0.40
1:A:476:ILE:HG12	1:A:517:VAL:HG11	2.04	0.40
1:A:49:TRP:CH2	1:A:436:PRO:HG3	2.55	0.40
1:A:124:PHE:CE1	1:A:174:LEU:HD12	2.56	0.40
2:B:107:TYR:HE2	2:B:109:GLN:NE2	2.19	0.40
1:A:271:GLN:CD	1:A:271:GLN:H	2.30	0.40
2:B:159:LYS:CB	2:B:162:LEU:HD12	2.52	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	512/529 (97%)	396 (77%)	71 (14%)	45 (9%)	0	9
2	B	215/230 (94%)	179 (83%)	26 (12%)	10 (5%)	2	16
All	All	727/759 (96%)	575 (79%)	97 (13%)	55 (8%)	1	10

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	PRO
1	A	106	VAL
1	A	111	ILE
1	A	121	GLN

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Mol	Chain	Res	Type
1	A	194	ILE
1	A	276	SER
1	A	412	HIS
1	A	445	PRO
1	A	458	HIS
1	A	466	SER
1	A	485	PRO
1	A	486	VAL
1	A	491	ALA
1	A	492	TRP
1	A	521	ARG
1	A	529	HIS
1	A	530	PRO
2	B	171	ASP
2	B	41	ASN
2	B	188	ASN
1	A	32	LEU
1	A	93	ALA
1	A	271	GLN
1	A	275	LYS
1	A	373	SER
1	A	446	LYS
1	A	493	GLN
1	A	506	TYR
1	A	532	PRO
2	B	158	CYS
1	A	24	MET
1	A	128	THR
1	A	376	PRO
2	B	30	GLU
2	B	31	PRO
2	B	165	THR
1	A	81	GLU
1	A	126	PRO
1	A	220	CYS
1	A	312	LYS
1	A	404	PHE
1	A	468	GLU
1	A	490	GLU
2	B	123	ARG
2	B	193	ASN
1	A	162	ILE

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Mol	Chain	Res	Type
2	B	13	ALA
1	A	525	GLY
1	A	378	PRO
1	A	436	PRO
1	A	475	PRO
1	A	509	PRO
1	A	377	LEU
1	A	526	GLY
1	A	282	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/457 (98%)	355 (80%)	91 (20%)	1	7
2	B	182/192 (95%)	160 (88%)	22 (12%)	5	18
All	All	628/649 (97%)	515 (82%)	113 (18%)	2	10

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	27	ILE
1	A	29	ILE
1	A	42	LEU
1	A	43	THR
1	A	49	TRP
1	A	56	THR
1	A	62	GLU
1	A	65	MET
1	A	73	GLU
1	A	74	VAL
1	A	87	VAL
1	A	94	SER
1	A	95	LYS

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Mol	Chain	Res	Type
1	A	96	ILE
1	A	101	PHE
1	A	106	VAL
1	A	109	GLU
1	A	112	ARG
1	A	115	THR
1	A	116	MET
1	A	123	SER
1	A	147	LEU
1	A	148	ILE
1	A	150	GLU
1	A	168	HIS
1	A	173	ILE
1	A	180	HIS
1	A	184	GLN
1	A	194	ILE
1	A	204	THR
1	A	206	LEU
1	A	207	ILE
1	A	209	ARG
1	A	219	GLU
1	A	223	LEU
1	A	227	CYS
1	A	235	GLU
1	A	236	ASP
1	A	255	CYS
1	A	256	GLU
1	A	257	LEU
1	A	267	ARG
1	A	269	SER
1	A	287	CYS
1	A	288	SER
1	A	311	CYS
1	A	315	CYS
1	A	316	SER
1	A	319	ASN
1	A	325	ARG
1	A	336	GLN
1	A	338	LEU
1	A	341	GLU
1	A	345	ILE
1	A	349	THR

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Mol	Chain	Res	Type
1	A	351	LYS
1	A	352	ILE
1	A	355	LEU
1	A	357	ASP
1	A	358	HIS
1	A	359	ILE
1	A	363	SER
1	A	367	ASN
1	A	373	SER
1	A	385	LEU
1	A	386	VAL
1	A	387	LYS
1	A	391	THR
1	A	401	THR
1	A	402	ASP
1	A	404	PHE
1	A	411	ILE
1	A	428	THR
1	A	433	VAL
1	A	443	VAL
1	A	458	HIS
1	A	465	ILE
1	A	481	LEU
1	A	483	TYR
1	A	488	HIS
1	A	489	TYR
1	A	495	ILE
1	A	496	GLN
1	A	497	VAL
1	A	498	THR
1	A	502	VAL
1	A	510	ARG
1	A	517	VAL
1	A	519	LEU
1	A	534	ARG
2	B	4	PHE
2	B	5	ARG
2	B	17	LYS
2	B	25	ILE
2	B	48	ILE
2	B	49	GLN
2	B	55	SER

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Mol	Chain	Res	Type
2	B	73	SER
2	B	108	SER
2	B	114	HIS
2	B	124	LEU
2	B	138	SER
2	B	139	LEU
2	B	145	ASP
2	B	150	ASP
2	B	162	LEU
2	B	181	MET
2	B	192	LEU
2	B	196	LYS
2	B	201	LYS
2	B	213	MET
2	B	218	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	68	HIS
1	A	76	GLN
1	A	140	ASN
1	A	214	GLN
1	A	230	ASN
1	A	297	GLN
1	A	318	ASN
1	A	336	GLN
1	A	438	ASN
1	A	449	ASN
1	A	459	ASN
2	B	49	GLN
2	B	71	ASN
2	B	109	GLN

5.3.3 RNA ⓘ

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	514/529 (97%)	0.81	62 (12%) 8 13	184, 225, 272, 309	0
2	B	217/230 (94%)	0.62	20 (9%) 14 18	191, 228, 268, 281	1 (0%)
All	All	731/759 (96%)	0.76	82 (11%) 10 15	184, 226, 270, 309	1 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	PRO	5.6
1	A	104	GLY	5.1
1	A	23	ALA	4.8
1	A	50	ARG	4.6
1	A	513	TYR	4.2
1	A	520	VAL	3.7
1	A	105	ARG	3.7
2	B	89	GLN	3.6
1	A	119	ARG	3.6
1	A	360	GLU	3.5
1	A	494	HIS	3.5
1	A	71	PRO	3.5
1	A	195	GLY	3.3
1	A	197	ASN	3.3
1	A	73	GLU	3.3
1	A	149	LYS	3.2
2	B	142	HIS	3.1
1	A	529	HIS	3.0
1	A	200	THR	3.0
1	A	467	SER	2.9
1	A	272	GLU	2.9
2	B	200	PHE	2.9
1	A	347	ARG	2.9
1	A	265	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	155	ASN	2.8
1	A	24	MET	2.8
1	A	354	ASP	2.8
1	A	497	VAL	2.8
1	A	402	ASP	2.7
1	A	62	GLU	2.7
1	A	518	GLN	2.7
1	A	524	GLU	2.7
2	B	41	ASN	2.7
2	B	127	LYS	2.6
1	A	357	ASP	2.6
1	A	183	PRO	2.6
1	A	499	ASN	2.6
1	A	514	GLU	2.6
1	A	412	HIS	2.6
1	A	267	ARG	2.5
1	A	442	LYS	2.5
1	A	107	ARG	2.5
1	A	295	GLY	2.5
1	A	344	GLY	2.5
1	A	399	ASN	2.5
1	A	498	THR	2.4
2	B	141	LEU	2.4
2	B	24	TYR	2.4
1	A	283	ASP	2.4
2	B	219	PHE	2.4
1	A	47	SER	2.4
1	A	355	LEU	2.4
1	A	108	GLY	2.3
1	A	392	VAL	2.3
1	A	396	LYS	2.3
2	B	174	GLY	2.3
1	A	527	GLU	2.3
2	B	201	LYS	2.3
2	B	198	HIS	2.3
1	A	229	ASN	2.3
1	A	271	GLN	2.3
1	A	486	VAL	2.2
2	B	135	LYS	2.2
1	A	184	GLN	2.2
1	A	230	ASN	2.2
1	A	490	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	203	PRO	2.1
1	A	468	GLU	2.1
2	B	56	LEU	2.1
1	A	128	THR	2.1
1	A	92	LYS	2.1
1	A	501	ILE	2.1
2	B	218	ASP	2.1
1	A	198	LEU	2.1
2	B	90	ARG	2.1
1	A	400	HIS	2.1
1	A	403	HIS	2.1
1	A	135	LYS	2.0
2	B	63	LYS	2.0
1	A	532	PRO	2.0
2	B	33	LYS	2.0
1	A	387	LYS	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.