



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:32 AM UTC

PDB ID : 5YWF / pdb_00005ywf
Title : Crystal structure of 2H4 Fab
Authors : Qiu, X.; Lei, Y.; Yang, P.; Gao, Q.; Wang, N.; Cao, L.; Wang, X.; Xu, Z.K.; Rao, Z.
Deposited on : 2017-11-29
Resolution : 2.21 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

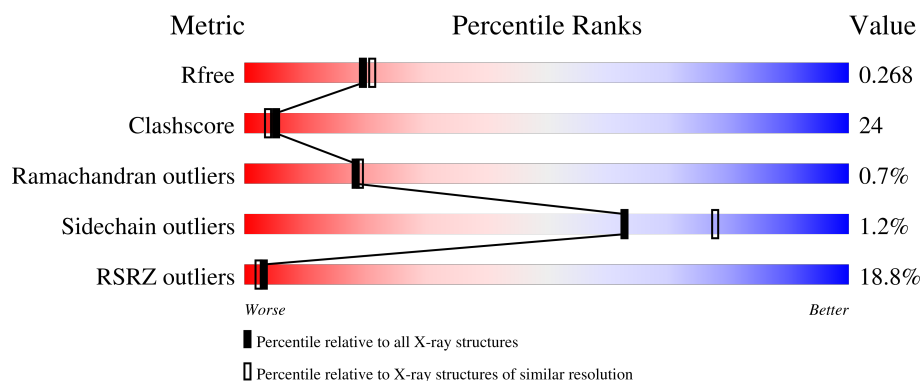
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	215	
1	C	215	
2	B	218	
2	D	218	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6772 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 2H4 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1657	1029	287	334	7			
1	C	215	Total	C	N	O	S	0	0	0
			1647	1022	283	336	6			

- Molecule 2 is a protein called 2H4 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1633	1041	264	320	8			
2	D	218	Total	C	N	O	S	0	0	0
			1628	1037	262	320	9			

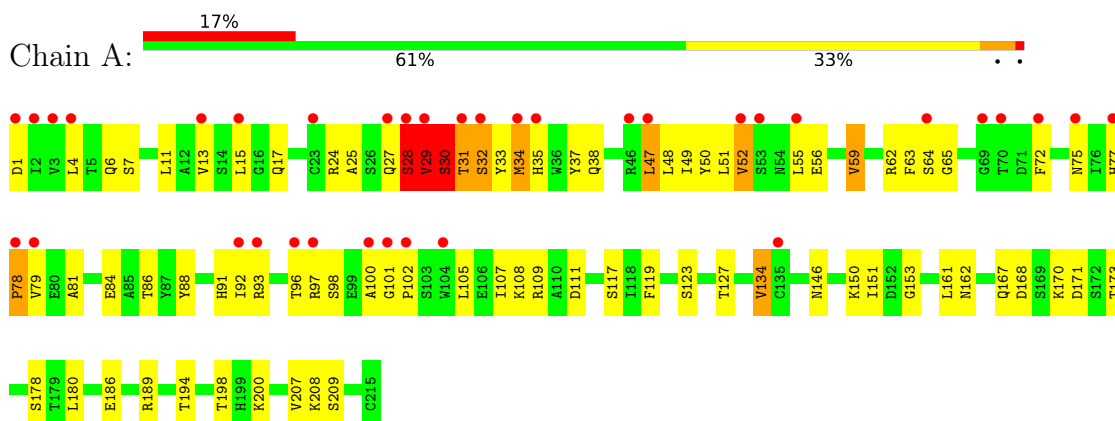
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	61	Total	O	0	0
			61	61		
3	C	46	Total	O	0	0
			46	46		
3	D	42	Total	O	0	0
			42	42		

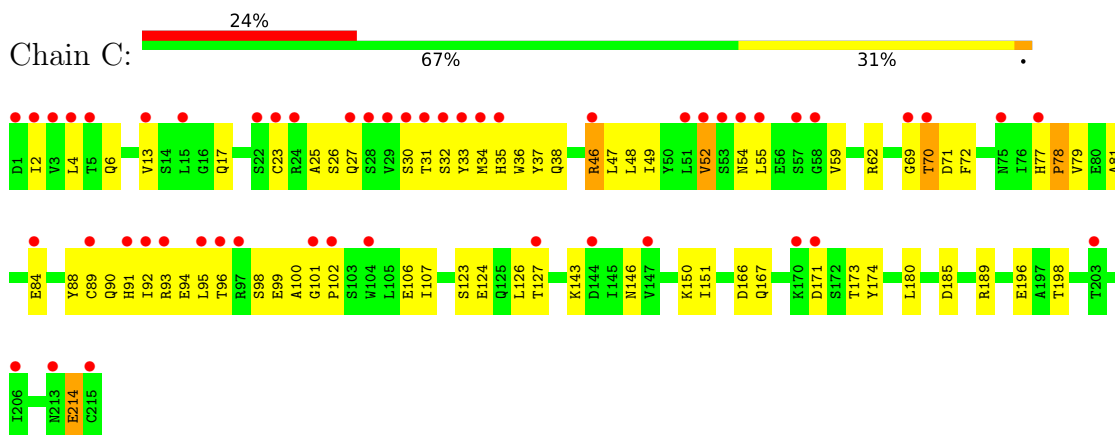
3 Residue-property plots [i](#)

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.

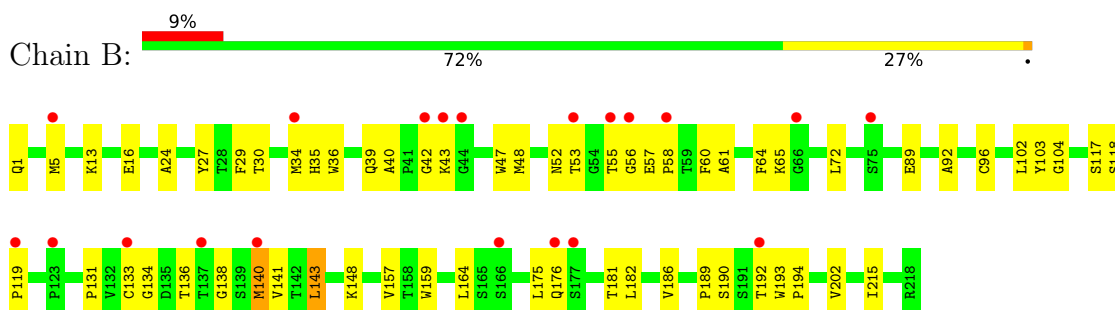
• Molecule 1: 2H4 light chain



• Molecule 1: 2H4 light chain

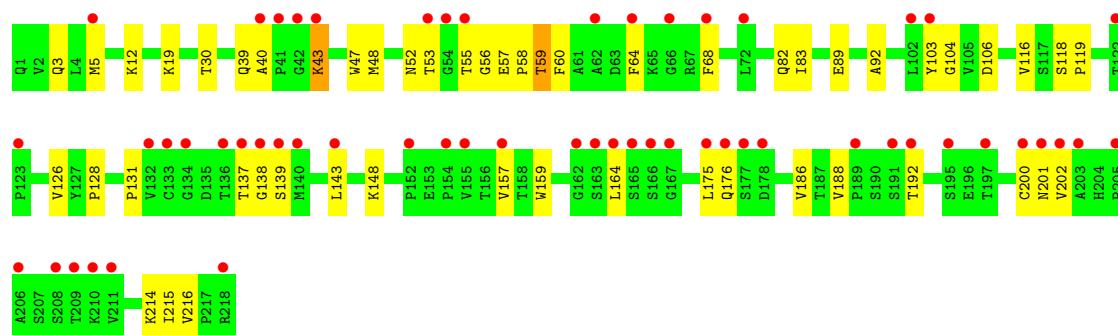


• Molecule 2: 2H4 heavy chain



● Molecule 2: 2H4 heavy chain

Chain D:  26% 76% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.37Å 140.98Å 78.96Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	44.36 – 2.21 44.36 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.36-2.21) 99.4 (44.36-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.215 , 0.262 0.233 , 0.268	Depositor DCC
R_{free} test set	2379 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6772	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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	0.61	1/1696 (0.1%)	0.89	3/2309 (0.1%)
1	C	0.63	4/1686 (0.2%)	0.83	4/2297 (0.2%)
2	B	0.43	0/1680	0.78	3/2299 (0.1%)
2	D	0.39	0/1675	0.74	1/2294 (0.0%)
All	All	0.53	5/6737 (0.1%)	0.81	11/9199 (0.1%)

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
2	B	0	1
2	D	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	ARG	NE-CZ	-12.33	1.19	1.33
1	C	46	ARG	CZ-NH2	-9.60	1.21	1.33
1	C	46	ARG	CD-NE	-9.21	1.33	1.46
1	C	46	ARG	CZ-NH1	-8.21	1.21	1.32
1	A	28	SER	CA-C	-6.19	1.44	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	VAL	N-CA-C	-11.48	85.47	109.34
1	C	70	THR	N-CA-C	9.25	121.36	111.28
1	A	32	SER	N-CA-C	-8.06	93.64	110.80
1	C	214	GLU	CA-C-N	7.24	134.73	121.70
1	C	214	GLU	C-N-CA	7.24	134.73	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	140	MET	N-CA-C	7.00	120.37	110.50
2	D	56	GLY	N-CA-C	-5.46	107.72	115.30
1	A	34	MET	CB-CG-SD	-5.43	96.39	112.70
1	C	93	ARG	N-CA-C	5.15	116.89	111.28
2	B	57	GLU	CA-C-N	5.03	125.42	119.99
2	B	57	GLU	C-N-CA	5.03	125.42	119.99

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	42	GLY	Peptide
2	D	43	LYS	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	1657	0	1573	133	0
1	C	1647	0	1549	89	1
2	B	1633	0	1585	81	0
2	D	1628	0	1570	52	1
3	A	58	0	0	2	0
3	B	61	0	0	4	0
3	C	46	0	0	6	0
3	D	42	0	0	1	0
All	All	6772	0	6277	311	1

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 24.

All (311) 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:34:MET:SD	1:A:72:PHE:CD1	2.05	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLY:O	1:C:72:PHE:CZ	1.67	1.44
1:C:69:GLY:O	1:C:72:PHE:CE1	1.95	1.18
1:A:31:THR:CG2	1:A:93:ARG:HH21	1.55	1.18
1:A:34:MET:SD	1:A:72:PHE:CE1	2.39	1.15
1:A:47:LEU:HD12	1:A:56:GLU:HG3	1.28	1.15
1:C:92:ILE:HD11	3:C:310:HOH:O	1.47	1.14
2:B:30:THR:HA	2:B:53:THR:CG2	1.77	1.13
1:C:4:LEU:HD11	1:C:91:HIS:CD2	1.90	1.06
1:C:4:LEU:HD11	1:C:91:HIS:HD2	1.20	1.06
1:A:92:ILE:HG21	2:B:104:GLY:N	1.72	1.04
2:B:30:THR:HA	2:B:53:THR:HG21	1.39	1.02
1:C:31:THR:H	1:C:69:GLY:HA2	1.26	1.00
1:C:96:THR:HG1	2:D:47:TRP:HE3	1.10	1.00
2:D:30:THR:HA	2:D:53:THR:OG1	1.62	0.99
1:C:31:THR:N	1:C:69:GLY:HA2	1.77	0.98
1:A:31:THR:CG2	1:A:93:ARG:NH2	2.25	0.98
1:A:4:LEU:HD11	1:A:91:HIS:HD2	1.28	0.97
1:A:35:HIS:ND1	3:A:301:HOH:O	1.96	0.97
1:A:34:MET:CE	1:A:72:PHE:CE1	2.48	0.96
1:C:69:GLY:O	1:C:72:PHE:HZ	1.32	0.95
2:B:148:LYS:HA	2:B:181:THR:HG22	1.47	0.94
2:D:148:LYS:NZ	2:D:176:GLN:HE22	1.63	0.94
1:C:92:ILE:CD1	3:C:310:HOH:O	2.06	0.93
1:A:15:LEU:CD2	2:D:139:SER:HB3	1.99	0.93
2:B:30:THR:HA	2:B:53:THR:HG22	1.55	0.89
1:C:92:ILE:HG21	2:D:104:GLY:N	1.88	0.89
1:A:31:THR:HG21	1:A:93:ARG:HH21	1.33	0.89
1:A:4:LEU:HD11	1:A:91:HIS:CD2	2.07	0.89
1:C:96:THR:OG1	2:D:47:TRP:HE3	1.53	0.89
2:B:133:CYS:O	3:B:301:HOH:O	1.92	0.87
1:C:91:HIS:CD2	1:C:98:SER:OG	2.28	0.86
1:A:92:ILE:HG21	2:B:104:GLY:H	1.36	0.86
1:C:96:THR:OG1	2:D:47:TRP:CE3	2.29	0.85
1:C:77:HIS:ND1	1:C:78:PRO:HD3	1.91	0.85
1:A:37:TYR:CE2	1:A:47:LEU:HD23	2.11	0.84
1:A:77:HIS:CG	1:A:78:PRO:HD3	2.14	0.83
1:A:97:ARG:HG2	1:A:97:ARG:HH21	1.40	0.83
1:A:111:ASP:OD2	1:A:200:LYS:NZ	2.11	0.82
1:C:55:LEU:HD12	1:C:55:LEU:O	1.80	0.81
1:A:97:ARG:HE	2:B:35:HIS:CE1	1.98	0.81
1:A:34:MET:SD	1:A:72:PHE:HD1	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:CYS:HG	1:C:89:CYS:HG	0.97	0.80
1:C:77:HIS:CG	1:C:78:PRO:HD3	2.16	0.80
1:A:91:HIS:CD2	1:A:98:SER:OG	2.36	0.79
1:A:107:ILE:H	1:A:167:GLN:HE22	1.31	0.78
2:D:148:LYS:HZ1	2:D:176:GLN:HE22	1.27	0.78
1:A:47:LEU:HD12	1:A:56:GLU:CG	2.12	0.78
1:A:34:MET:HE1	1:A:72:PHE:HE1	1.50	0.77
1:A:15:LEU:HD21	2:D:139:SER:CB	2.16	0.75
1:A:34:MET:HE1	1:A:72:PHE:CE1	2.22	0.75
1:C:88:TYR:CE1	1:C:102:PRO:HB3	2.21	0.74
1:C:35:HIS:CE1	1:C:47:LEU:HD21	2.22	0.74
1:C:35:HIS:NE2	2:D:103:TYR:O	2.21	0.74
1:A:96:THR:HG22	2:B:47:TRP:HZ3	1.54	0.73
1:A:29:VAL:C	1:A:31:THR:H	1.96	0.73
1:A:108:LYS:O	2:D:138:GLY:HA3	1.89	0.73
1:C:4:LEU:CD1	1:C:91:HIS:HD2	2.00	0.72
1:A:35:HIS:CE1	2:B:103:TYR:O	2.43	0.72
1:A:208:LYS:HE3	2:B:134:GLY:O	1.90	0.72
1:A:15:LEU:CD2	2:D:139:SER:CB	2.67	0.71
2:D:175:LEU:C	2:D:175:LEU:HD23	2.14	0.71
2:B:148:LYS:HG3	2:B:181:THR:CG2	2.20	0.71
1:A:15:LEU:HD23	2:D:139:SER:HB3	1.72	0.71
2:B:176:GLN:NE2	2:B:181:THR:OG1	2.23	0.70
1:A:77:HIS:ND1	1:A:78:PRO:HD3	2.06	0.70
1:A:171:ASP:OD2	1:A:173:THR:OG1	2.10	0.69
1:A:96:THR:HB	2:B:47:TRP:CE3	2.28	0.69
2:B:34:MET:HE1	2:B:96:CYS:HB2	1.73	0.69
1:C:91:HIS:CD2	1:C:98:SER:HG	2.09	0.68
1:A:92:ILE:CD1	2:B:104:GLY:HA3	2.24	0.68
2:B:52:ASN:HD22	2:B:55:THR:HB	1.59	0.68
2:D:40:ALA:HB3	2:D:43:LYS:H	1.58	0.68
1:C:185:ASP:O	1:C:189:ARG:HG3	1.95	0.67
1:A:194:THR:OG1	1:A:209:SER:HB2	1.95	0.67
1:A:123:SER:O	1:A:127:THR:HG23	1.95	0.67
2:B:29:PHE:O	2:B:53:THR:HG21	1.94	0.67
2:B:141:VAL:HG13	2:B:190:SER:HB3	1.75	0.67
1:A:86:THR:HG22	1:A:102:PRO:HB2	1.76	0.66
1:A:31:THR:HG23	1:A:93:ARG:NH2	2.11	0.66
1:C:81:ALA:O	1:C:84:GLU:HG2	1.95	0.66
2:B:30:THR:CA	2:B:53:THR:HG21	2.22	0.66
2:B:36:TRP:HB3	2:B:48:MET:HE3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:HG22	1:A:93:ARG:NH2	2.10	0.66
1:A:37:TYR:CD2	1:A:47:LEU:HD23	2.32	0.65
1:A:49:ILE:CD1	1:A:55:LEU:HD23	2.27	0.65
2:B:131:PRO:HD3	2:B:143:LEU:HD12	1.79	0.64
1:A:91:HIS:NE2	1:A:98:SER:OG	2.30	0.64
2:B:157:VAL:HG22	2:B:202:VAL:HG22	1.79	0.64
1:A:92:ILE:HG13	2:B:103:TYR:C	2.23	0.63
1:A:15:LEU:HA	1:A:79:VAL:HG23	1.78	0.63
1:C:2:ILE:HG21	1:C:94:GLU:OE2	1.98	0.63
2:B:175:LEU:O	2:B:176:GLN:HG3	1.98	0.63
2:D:148:LYS:HZ2	2:D:176:GLN:HE22	1.45	0.63
1:A:55:LEU:HD21	1:A:63:PHE:O	1.99	0.62
1:A:34:MET:SD	1:A:72:PHE:CG	2.85	0.62
1:A:97:ARG:HH21	1:A:97:ARG:CG	2.11	0.62
1:A:93:ARG:O	1:A:93:ARG:HD3	1.99	0.62
1:A:92:ILE:HB	2:B:102:LEU:O	2.00	0.62
2:D:39:GLN:O	2:D:92:ALA:HB1	1.99	0.62
2:B:30:THR:OG1	3:B:302:HOH:O	2.16	0.62
2:B:159:TRP:HZ3	2:B:215:ILE:HD11	1.64	0.62
1:A:1:ASP:N	3:A:303:HOH:O	2.28	0.62
1:A:92:ILE:HD12	2:B:104:GLY:CA	2.30	0.62
2:B:175:LEU:C	2:B:176:GLN:HG3	2.25	0.61
1:A:168:ASP:OD1	1:A:170:LYS:HD2	2.01	0.61
1:A:92:ILE:HD12	2:B:104:GLY:HA3	1.83	0.61
1:C:32:SER:O	1:C:33:TYR:C	2.44	0.61
1:C:70:THR:HG23	1:C:71:ASP:OD1	2.00	0.61
1:A:27:GLN:HG3	1:A:28:SER:N	2.15	0.61
1:C:2:ILE:CG2	1:C:94:GLU:OE2	2.48	0.61
1:C:123:SER:O	1:C:127:THR:HG23	2.01	0.60
1:C:38:GLN:NE2	1:C:46:ARG:HH21	1.99	0.60
2:D:3:GLN:HB3	2:D:5:MET:SD	2.42	0.60
1:A:31:THR:OG1	1:A:32:SER:N	2.33	0.59
2:B:141:VAL:CG1	2:B:190:SER:HB3	2.32	0.59
1:A:34:MET:C	1:A:35:HIS:CD2	2.80	0.59
1:A:38:GLN:HB2	1:A:48:LEU:HD11	1.84	0.59
1:A:81:ALA:O	1:A:84:GLU:HG2	2.02	0.59
1:C:37:TYR:CE2	1:C:47:LEU:HD13	2.37	0.59
1:A:48:LEU:HA	1:A:59:VAL:HG11	1.83	0.59
1:A:119:PHE:HB2	1:A:134:VAL:HG22	1.84	0.58
1:C:91:HIS:NE2	1:C:98:SER:OG	2.23	0.58
1:C:69:GLY:C	1:C:72:PHE:CZ	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:LYS:N	2:B:16:GLU:OE1	2.25	0.58
1:C:150:LYS:NZ	1:C:196:GLU:OE1	2.23	0.58
1:C:2:ILE:HG13	1:C:26:SER:OG	2.04	0.57
1:C:38:GLN:HE22	1:C:46:ARG:HH21	1.52	0.57
1:A:29:VAL:HG12	1:A:29:VAL:O	2.03	0.57
2:B:56:GLY:HA2	2:B:72:LEU:HD11	1.85	0.57
1:C:146:ASN:HB3	1:C:198:THR:CG2	2.34	0.57
2:D:19:LYS:HD3	2:D:82:GLN:HB2	1.87	0.57
2:B:148:LYS:HG3	2:B:181:THR:HG21	1.86	0.56
1:C:37:TYR:CD2	1:C:47:LEU:HD13	2.41	0.56
2:D:131:PRO:HD3	2:D:143:LEU:HD22	1.87	0.56
1:A:108:LYS:O	2:D:138:GLY:CA	2.52	0.56
2:B:55:THR:O	2:B:55:THR:HG22	2.04	0.56
1:C:32:SER:O	1:C:34:MET:N	2.39	0.56
2:B:176:GLN:OE1	2:B:181:THR:HG23	2.05	0.56
1:C:171:ASP:OD2	1:C:173:THR:OG1	2.21	0.56
1:A:13:VAL:HG23	1:A:17:GLN:NE2	2.21	0.55
1:C:2:ILE:HA	1:C:26:SER:OG	2.06	0.55
1:A:4:LEU:CD1	1:A:91:HIS:HD2	2.11	0.55
1:A:47:LEU:HD13	1:A:48:LEU:N	2.21	0.55
1:C:106:GLU:HG2	1:C:107:ILE:N	2.21	0.55
1:C:30:SER:HB3	1:C:69:GLY:C	2.32	0.55
1:C:31:THR:H	1:C:69:GLY:CA	2.11	0.55
1:A:194:THR:OG1	1:A:209:SER:CB	2.54	0.54
1:C:13:VAL:CG2	1:C:79:VAL:HG11	2.38	0.54
1:C:47:LEU:HD22	2:D:106:ASP:HA	1.88	0.54
2:B:34:MET:CE	2:B:96:CYS:HB2	2.38	0.54
1:A:27:GLN:CG	1:A:28:SER:N	2.71	0.54
1:C:77:HIS:CE1	1:C:78:PRO:HD3	2.42	0.53
1:C:146:ASN:HB3	1:C:198:THR:HG22	1.89	0.53
2:D:126:VAL:HG21	2:D:202:VAL:HG21	1.89	0.53
1:A:146:ASN:HB3	1:A:198:THR:HG22	1.90	0.53
2:B:36:TRP:CB	2:B:48:MET:HE3	2.39	0.53
1:A:146:ASN:HB3	1:A:198:THR:CG2	2.39	0.53
2:B:159:TRP:HZ3	2:B:215:ILE:CD1	2.21	0.53
2:B:36:TRP:HB3	2:B:48:MET:CE	2.37	0.53
1:C:55:LEU:HD12	1:C:55:LEU:C	2.33	0.52
2:B:148:LYS:HG3	2:B:181:THR:HG22	1.90	0.52
2:B:89:GLU:N	2:B:89:GLU:OE2	2.43	0.52
2:B:159:TRP:CZ3	2:B:215:ILE:HD11	2.43	0.52
1:A:97:ARG:CG	1:A:97:ARG:NH2	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:HB3	1:A:59:VAL:HG22	1.92	0.51
2:B:138:GLY:HA2	1:C:107:ILE:HG12	1.92	0.51
1:C:124:GLU:OE2	1:C:124:GLU:N	2.44	0.51
2:D:157:VAL:HG22	2:D:202:VAL:HG12	1.92	0.51
1:A:161:LEU:CD1	2:B:176:GLN:HG2	2.41	0.51
1:A:92:ILE:HG21	2:B:104:GLY:CA	2.40	0.50
1:A:96:THR:HB	2:B:47:TRP:HE3	1.76	0.50
1:A:84:GLU:OE1	1:A:107:ILE:HB	2.12	0.50
1:C:36:TRP:O	1:C:47:LEU:HD12	2.11	0.50
2:D:89:GLU:CD	2:D:89:GLU:H	2.20	0.50
1:A:34:MET:C	1:A:35:HIS:HD2	2.19	0.50
1:A:92:ILE:CG2	2:B:104:GLY:N	2.59	0.50
2:B:61:ALA:O	2:B:65:LYS:HG3	2.12	0.50
2:B:136:THR:HG23	2:B:141:VAL:HG12	1.93	0.50
1:A:151:ILE:HD11	1:A:180:LEU:HD21	1.94	0.50
1:A:97:ARG:HE	2:B:35:HIS:HE1	1.53	0.50
1:A:171:ASP:OD1	1:A:171:ASP:N	2.37	0.50
1:A:49:ILE:HD11	1:A:55:LEU:HD23	1.94	0.50
2:D:148:LYS:HZ1	2:D:176:GLN:NE2	2.02	0.50
2:D:12:LYS:O	2:D:116:VAL:HA	2.13	0.49
1:A:86:THR:CG2	1:A:102:PRO:HB2	2.41	0.49
2:B:48:MET:HA	2:B:64:PHE:CD2	2.47	0.49
2:D:30:THR:HA	2:D:53:THR:HG1	1.76	0.49
1:C:38:GLN:NE2	1:C:46:ARG:NH2	2.59	0.49
2:D:68:PHE:CD2	2:D:83:ILE:HG12	2.48	0.49
2:B:48:MET:HG2	2:B:64:PHE:CZ	2.48	0.49
1:C:90:GLN:CB	3:C:341:HOH:O	2.60	0.49
2:D:118:SER:N	2:D:119:PRO:HD3	2.27	0.49
1:C:38:GLN:HE22	1:C:46:ARG:NH2	2.11	0.48
1:A:7:SER:HB3	1:A:24:ARG:HH22	1.78	0.48
2:D:148:LYS:NZ	2:D:176:GLN:NE2	2.47	0.48
1:A:6:GLN:HB2	1:A:101:GLY:O	2.14	0.48
2:B:193:TRP:CG	2:B:194:PRO:HA	2.48	0.48
2:D:164:LEU:HD13	2:D:186:VAL:HG21	1.96	0.47
1:C:151:ILE:HD11	1:C:180:LEU:HD21	1.96	0.47
2:B:52:ASN:HD22	2:B:55:THR:CB	2.26	0.47
1:C:36:TRP:CZ3	1:C:89:CYS:HB3	2.49	0.47
2:D:128:PRO:HB3	2:D:215:ILE:HD13	1.97	0.47
1:A:35:HIS:CE1	1:A:50:TYR:HA	2.50	0.47
1:C:46:ARG:NH1	3:C:308:HOH:O	2.47	0.47
1:A:150:LYS:NZ	1:A:153:GLY:O	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TYR:CE2	1:A:102:PRO:HB3	2.50	0.47
1:C:92:ILE:HG21	2:D:104:GLY:H	1.74	0.47
2:B:39:GLN:NE2	3:B:306:HOH:O	2.48	0.46
1:C:4:LEU:HD23	1:C:25:ALA:HA	1.97	0.46
1:A:34:MET:HB2	1:A:34:MET:HE3	1.30	0.46
1:C:6:GLN:HG3	1:C:100:ALA:HB3	1.96	0.46
1:C:95:LEU:N	1:C:95:LEU:HD12	2.31	0.46
1:A:77:HIS:CE1	1:A:78:PRO:HD3	2.50	0.46
1:C:62:ARG:HA	1:C:77:HIS:ND1	2.31	0.46
2:B:1:GLN:N	2:B:1:GLN:CD	2.74	0.46
1:A:92:ILE:HG22	1:A:92:ILE:O	2.16	0.46
1:C:48:LEU:HA	1:C:59:VAL:HG21	1.98	0.46
2:D:188:VAL:CG1	2:D:192:THR:HB	2.46	0.46
1:A:15:LEU:HD21	2:D:139:SER:HB2	1.95	0.46
1:A:162:ASN:HD22	1:A:178:SER:HA	1.81	0.46
2:B:1:GLN:CD	2:B:1:GLN:H3	2.24	0.45
1:C:6:GLN:HG3	1:C:100:ALA:CB	2.46	0.45
1:C:13:VAL:HG21	1:C:79:VAL:HG11	1.96	0.45
1:A:4:LEU:HD23	1:A:25:ALA:HA	1.98	0.45
1:A:35:HIS:ND1	1:A:50:TYR:HA	2.31	0.45
1:C:2:ILE:HG23	1:C:2:ILE:O	2.15	0.45
1:A:55:LEU:HD22	1:A:59:VAL:CG2	2.47	0.45
1:A:92:ILE:CG2	2:B:104:GLY:CA	2.94	0.45
2:B:136:THR:HG23	2:B:140:MET:O	2.16	0.45
2:D:48:MET:HA	2:D:64:PHE:CD2	2.52	0.45
1:A:30:SER:HA	1:A:93:ARG:HG2	1.97	0.45
1:C:88:TYR:CZ	1:C:102:PRO:HB3	2.51	0.45
1:A:27:GLN:CG	1:A:28:SER:H	2.29	0.45
2:D:55:THR:HG22	2:D:57:GLU:HB2	1.98	0.45
2:D:214:LYS:HG2	2:D:216:VAL:HG13	1.99	0.45
1:A:107:ILE:HD11	2:D:139:SER:OG	2.17	0.45
1:A:93:ARG:HD3	1:A:93:ARG:C	2.41	0.45
2:B:5:MET:O	2:B:5:MET:HG3	2.16	0.45
1:C:143:LYS:HE2	1:C:143:LYS:HB2	1.68	0.45
1:A:6:GLN:HG3	1:A:100:ALA:CB	2.47	0.45
2:B:58:PRO:HB2	2:B:60:PHE:CE2	2.51	0.45
1:A:17:GLN:O	1:A:79:VAL:HG22	2.17	0.44
1:C:6:GLN:HB2	1:C:101:GLY:O	2.17	0.44
1:C:52:VAL:CB	3:C:318:HOH:O	2.65	0.44
1:A:13:VAL:HG23	1:A:17:GLN:CD	2.41	0.44
1:A:92:ILE:HD12	2:B:104:GLY:HA2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:PRO:HG2	2:B:192:THR:HG23	1.99	0.44
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.80	0.44
1:A:29:VAL:C	1:A:31:THR:N	2.69	0.44
2:B:118:SER:N	2:B:119:PRO:HD3	2.33	0.44
2:D:59:THR:HG23	3:D:317:HOH:O	2.17	0.44
2:D:175:LEU:C	2:D:175:LEU:CD2	2.85	0.44
2:B:24:ALA:HB1	2:B:27:TYR:CE1	2.52	0.44
2:D:52:ASN:HB3	2:D:55:THR:HB	1.99	0.44
2:D:55:THR:CG2	2:D:57:GLU:HB2	2.47	0.44
1:A:194:THR:HG23	1:A:208:LYS:O	2.17	0.44
1:C:35:HIS:HE1	1:C:47:LEU:HD21	1.77	0.44
1:C:2:ILE:CG2	1:C:91:HIS:NE2	2.81	0.44
1:A:29:VAL:O	1:A:31:THR:N	2.50	0.44
1:A:35:HIS:HE1	2:B:103:TYR:HB3	1.82	0.44
1:C:90:GLN:CB	1:C:99:GLU:HG3	2.48	0.44
2:D:55:THR:HG22	2:D:57:GLU:CB	2.48	0.44
1:A:194:THR:CG2	1:A:207:VAL:HG13	2.48	0.44
1:A:37:TYR:CE2	1:A:47:LEU:CD2	2.93	0.43
1:A:91:HIS:O	1:A:91:HIS:CG	2.70	0.43
1:C:91:HIS:O	1:C:91:HIS:CG	2.70	0.43
2:D:55:THR:CG2	2:D:57:GLU:CB	2.96	0.43
1:A:52:VAL:O	1:A:65:GLY:C	2.61	0.43
2:B:40:ALA:HB3	2:B:43:LYS:CB	2.48	0.43
2:D:57:GLU:HA	2:D:58:PRO:HD3	1.88	0.43
2:B:56:GLY:HA2	2:B:72:LEU:CD1	2.48	0.43
1:A:35:HIS:CE1	2:B:103:TYR:HB3	2.53	0.43
1:A:97:ARG:NE	2:B:35:HIS:CE1	2.78	0.43
1:C:23:CYS:CB	1:C:89:CYS:SG	3.06	0.43
1:A:96:THR:CG2	2:B:47:TRP:HZ3	2.27	0.43
2:B:39:GLN:O	2:B:92:ALA:HB1	2.19	0.43
1:A:92:ILE:HG13	2:B:104:GLY:HA3	2.00	0.43
1:A:35:HIS:CE1	1:A:50:TYR:HB2	2.53	0.42
1:A:47:LEU:CD1	1:A:56:GLU:HG3	2.21	0.42
2:D:157:VAL:HA	2:D:201:ASN:O	2.19	0.42
1:A:92:ILE:CG1	2:B:104:GLY:HA3	2.49	0.42
1:C:2:ILE:HD12	1:C:27:GLN:CB	2.50	0.42
1:C:17:GLN:O	1:C:79:VAL:HG12	2.20	0.42
1:A:32:SER:HB3	1:A:51:LEU:O	2.19	0.42
1:A:62:ARG:HA	1:A:77:HIS:ND1	2.33	0.42
2:B:117:SER:HB2	2:B:119:PRO:HD3	2.01	0.42
2:D:48:MET:HG2	2:D:64:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ILE:HA	1:C:54:ASN:O	2.19	0.42
1:A:96:THR:HB	2:B:47:TRP:CZ3	2.54	0.42
1:A:31:THR:OG1	1:A:33:TYR:CD2	2.71	0.42
1:C:166:ASP:CG	1:C:167:GLN:H	2.28	0.42
1:C:47:LEU:HD12	1:C:48:LEU:H	1.85	0.42
1:A:13:VAL:HG22	1:A:79:VAL:HG21	2.02	0.41
1:A:92:ILE:HG13	2:B:104:GLY:N	2.34	0.41
1:C:2:ILE:HG22	1:C:94:GLU:OE2	2.19	0.41
1:C:47:LEU:CD2	2:D:106:ASP:HA	2.51	0.41
2:D:60:PHE:CE1	2:D:68:PHE:O	2.73	0.41
1:C:69:GLY:O	1:C:72:PHE:HE1	1.85	0.41
1:C:174:TYR:HB3	3:C:315:HOH:O	2.21	0.41
1:A:109:ARG:HD2	1:A:171:ASP:O	2.20	0.41
1:A:186:GLU:O	1:A:189:ARG:HG2	2.21	0.41
2:B:182:LEU:HA	3:B:317:HOH:O	2.20	0.41
2:D:159:TRP:CZ3	2:D:200:CYS:HB3	2.55	0.41
1:A:47:LEU:HD22	1:A:47:LEU:HA	1.80	0.41
1:A:64:SER:HB3	1:A:75:ASN:HB3	2.01	0.41
2:B:164:LEU:HD13	2:B:186:VAL:HG21	2.03	0.41
1:A:11:LEU:HD22	1:A:105:LEU:HD11	2.02	0.40
1:C:92:ILE:O	1:C:92:ILE:HG22	2.21	0.40
1:A:117:SER:HB3	1:A:119:PHE:CE1	2.56	0.40
1:C:171:ASP:OD1	1:C:171:ASP:N	2.46	0.40

All (1) 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:C:214:GLU:OE1	2:D:53:THR:CG2[2_745]	2.18	0.02

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	213/215 (99%)	199 (93%)	10 (5%)	4 (2%)	6	4
1	C	213/215 (99%)	201 (94%)	10 (5%)	2 (1%)	14	14
2	B	216/218 (99%)	205 (95%)	11 (5%)	0	100	100
2	D	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
All	All	858/866 (99%)	811 (94%)	41 (5%)	6 (1%)	18	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	52	VAL
1	A	78	PRO
1	C	52	VAL
1	C	78	PRO
1	A	30	SER

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	186/192 (97%)	180 (97%)	6 (3%)	34	47
1	C	184/192 (96%)	184 (100%)	0	100	100
2	B	183/185 (99%)	182 (100%)	1 (0%)	81	90
2	D	182/185 (98%)	180 (99%)	2 (1%)	65	79
All	All	735/754 (98%)	726 (99%)	9 (1%)	63	78

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	30	SER
1	A	31	THR
1	A	47	LEU
1	A	59	VAL

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Mol	Chain	Res	Type
1	A	134	VAL
2	B	143	LEU
2	D	59	THR
2	D	137	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	39	GLN
1	A	75	ASN
1	A	162	ASN
1	A	167	GLN
1	A	213	ASN
2	B	39	GLN
2	B	52	ASN
2	B	176	GLN
1	C	38	GLN
1	C	39	GLN
1	C	190	HIS
1	C	191	ASN
2	D	39	GLN
2	D	176	GLN
2	D	201	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	215/215 (100%)	0.90	36 (16%) 4 3	24, 41, 60, 86	0
1	C	215/215 (100%)	1.29	51 (23%) 2 1	26, 50, 77, 102	0
2	B	218/218 (100%)	0.60	20 (9%) 14 12	23, 39, 63, 74	0
2	D	218/218 (100%)	1.23	56 (25%) 1 1	31, 50, 83, 92	0
All	All	866/866 (100%)	1.01	163 (18%) 3 2	23, 45, 75, 102	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	VAL	6.7
1	A	28	SER	6.5
1	C	55	LEU	6.1
1	C	29	VAL	5.5
1	C	28	SER	5.5
1	A	29	VAL	5.5
1	C	52	VAL	5.5
1	C	31	THR	5.3
2	D	5	MET	5.2
1	C	69	GLY	5.1
1	C	30	SER	5.0
1	A	104	TRP	5.0
1	A	92	ILE	4.9
1	C	2	ILE	4.9
2	B	44	GLY	4.7
1	C	104	TRP	4.6
1	A	34	MET	4.4
1	C	92	ILE	4.3
2	D	155	VAL	4.3
1	A	31	THR	4.2
2	D	175	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	206	ALA	4.2
1	A	102	PRO	4.2
2	B	5	MET	4.2
1	C	1	ASP	4.1
1	C	101	GLY	4.1
1	C	215	CYS	4.1
2	D	157	VAL	4.0
2	D	209	THR	4.0
1	C	102	PRO	4.0
1	A	97	ARG	4.0
2	D	139	SER	4.0
2	D	164	LEU	3.9
2	D	178	ASP	3.7
2	D	166	SER	3.7
2	D	162	GLY	3.7
2	D	53	THR	3.7
1	A	101	GLY	3.6
2	D	103	TYR	3.6
2	D	197	THR	3.5
1	C	34	MET	3.4
1	A	2	ILE	3.3
1	C	84	GLU	3.3
1	C	93	ARG	3.3
2	D	202	VAL	3.3
1	A	93	ARG	3.3
1	A	69	GLY	3.3
2	D	140	MET	3.3
2	D	210	LYS	3.3
2	B	75	SER	3.2
2	D	176	GLN	3.2
2	B	66	GLY	3.2
2	D	66	GLY	3.2
1	C	96	THR	3.1
1	C	27	GLN	3.1
1	C	57	SER	3.1
2	B	177	SER	3.1
1	A	55	LEU	3.1
2	D	40	ALA	3.1
1	C	75	ASN	3.0
2	D	133	CYS	3.0
1	A	77	HIS	3.0
1	C	35	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	53	SER	3.0
2	B	166	SER	3.0
2	D	123	PRO	2.9
2	D	165	SER	2.9
1	A	72	PHE	2.9
1	A	96	THR	2.9
2	B	53	THR	2.9
1	C	32	SER	2.8
2	D	177	SER	2.8
2	B	176	GLN	2.8
1	C	13	VAL	2.8
2	D	211	VAL	2.8
2	D	55	THR	2.8
1	A	100	ALA	2.8
1	C	203	THR	2.8
2	D	192	THR	2.8
2	D	43	LYS	2.8
2	B	133	CYS	2.7
1	C	46	ARG	2.7
1	A	75	ASN	2.7
1	C	54	ASN	2.7
2	D	138	GLY	2.7
2	B	43	LYS	2.7
1	A	79	VAL	2.7
2	B	123	PRO	2.7
1	C	77	HIS	2.6
1	C	95	LEU	2.6
2	B	56	GLY	2.6
1	C	22	SER	2.6
1	A	35	HIS	2.6
2	D	54	GLY	2.6
1	C	4	LEU	2.5
2	B	140	MET	2.5
2	B	42	GLY	2.5
2	D	136	THR	2.5
1	C	91	HIS	2.5
2	D	154	PRO	2.5
1	C	127	THR	2.5
2	B	55	THR	2.5
2	D	102	LEU	2.5
1	C	53	SER	2.4
1	A	13	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	203	ALA	2.4
2	D	137	THR	2.4
2	D	64	PHE	2.4
1	C	3	VAL	2.4
2	D	68	PHE	2.4
1	A	47	LEU	2.4
1	A	1	ASP	2.4
1	C	171	ASP	2.4
1	C	170	LYS	2.4
2	D	191	SER	2.4
1	C	89	CYS	2.4
1	A	15	LEU	2.4
2	D	72	LEU	2.4
1	C	24	ARG	2.4
1	C	70	THR	2.3
1	A	3	VAL	2.3
1	A	135	CYS	2.3
1	C	147	VAL	2.3
1	C	97	ARG	2.3
1	A	27	GLN	2.3
1	C	23	CYS	2.3
2	B	119	PRO	2.3
1	A	70	THR	2.3
2	D	163	SER	2.3
2	D	167	GLY	2.3
2	D	62	ALA	2.3
1	A	23	CYS	2.2
2	D	41	PRO	2.2
2	D	42	GLY	2.2
1	C	33	TYR	2.2
1	C	15	LEU	2.2
2	D	200	CYS	2.2
1	C	5	THR	2.2
1	A	4	LEU	2.2
2	D	122	THR	2.2
1	A	78	PRO	2.1
1	A	64	SER	2.1
2	B	137	THR	2.1
2	D	218	ARG	2.1
1	C	206	ILE	2.1
2	D	143	LEU	2.1
2	D	201	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	189	PRO	2.1
1	C	58	GLY	2.1
2	B	192	THR	2.1
1	C	144	ASP	2.1
2	D	152	PRO	2.1
2	D	205	PRO	2.1
2	D	195	SER	2.1
2	B	58	PRO	2.1
2	B	34	MET	2.0
1	C	51	LEU	2.0
2	D	132	VAL	2.0
2	D	134	GLY	2.0
1	A	32	SER	2.0
2	D	208	SER	2.0
1	C	213	ASN	2.0
1	A	46	ARG	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.