



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:46 PM UTC

PDB ID : 8PWV / pdb_00008pwv
Title : PfRH5 bound to monoclonal antibody MAD8-502
Authors : Farrell, B.; Higgins, M.K.
Deposited on : 2023-07-21
Resolution : 2.07 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

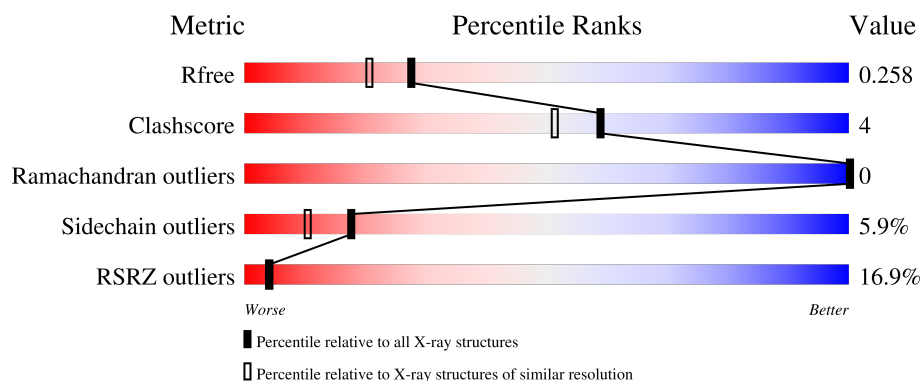
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	338	16% 72% 10% • 16%
1	C	338	12% 72% 10% • 16%
1	E	338	20% 66% 14% • 16%
1	G	338	17% 69% 13% • 17%
2	B	252	6% 77% 11% • 10%

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Mol	Chain	Length	Quality of chain
2	D	252	13% 79% 10% • 10%
2	F	252	22% 76% 13% • 10%
2	H	252	9% 78% 10% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16925 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 Reticulocyte-binding protein homolog 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2414	1559	405	437	13			
1	C	284	Total	C	N	O	S	0	0	0
			2414	1559	405	437	13			
1	E	283	Total	C	N	O	S	0	0	0
			2405	1554	403	435	13			
1	G	281	Total	C	N	O	S	0	0	0
			2390	1545	400	432	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	TYR	CYS	engineered mutation	UNP Q8IFM5
A	216	ALA	THR	engineered mutation	UNP Q8IFM5
A	299	ALA	THR	engineered mutation	UNP Q8IFM5
C	203	TYR	CYS	engineered mutation	UNP Q8IFM5
C	216	ALA	THR	engineered mutation	UNP Q8IFM5
C	299	ALA	THR	engineered mutation	UNP Q8IFM5
E	203	TYR	CYS	engineered mutation	UNP Q8IFM5
E	216	ALA	THR	engineered mutation	UNP Q8IFM5
E	299	ALA	THR	engineered mutation	UNP Q8IFM5
G	203	TYR	CYS	engineered mutation	UNP Q8IFM5
G	216	ALA	THR	engineered mutation	UNP Q8IFM5
G	299	ALA	THR	engineered mutation	UNP Q8IFM5

- Molecule 2 is a protein called monoclonal antibody MAD8-502.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1725	1090	288	338	9			
2	D	227	Total	C	N	O	S	0	1	0
			1725	1090	287	339	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	226	Total	C	N	O	S	0	1	0
			1716	1084	285	338	9			
2	H	226	Total	C	N	O	S	0	1	0
			1718	1085	286	338	9			

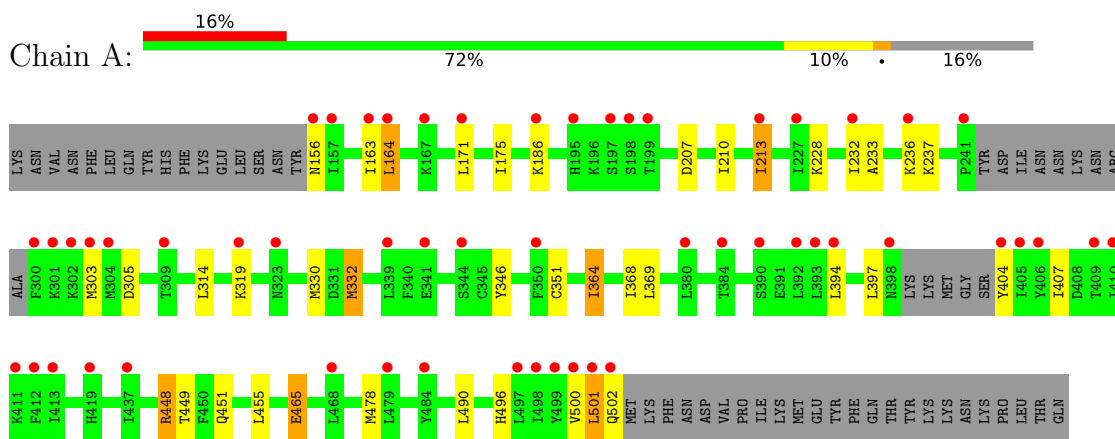
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total	O	0	0
			43	43		
3	B	92	Total	O	0	0
			92	92		
3	C	69	Total	O	0	0
			69	69		
3	D	37	Total	O	0	0
			37	37		
3	E	102	Total	O	0	0
			102	102		
3	F	30	Total	O	0	0
			30	30		
3	G	10	Total	O	0	0
			10	10		
3	H	35	Total	O	0	0
			35	35		

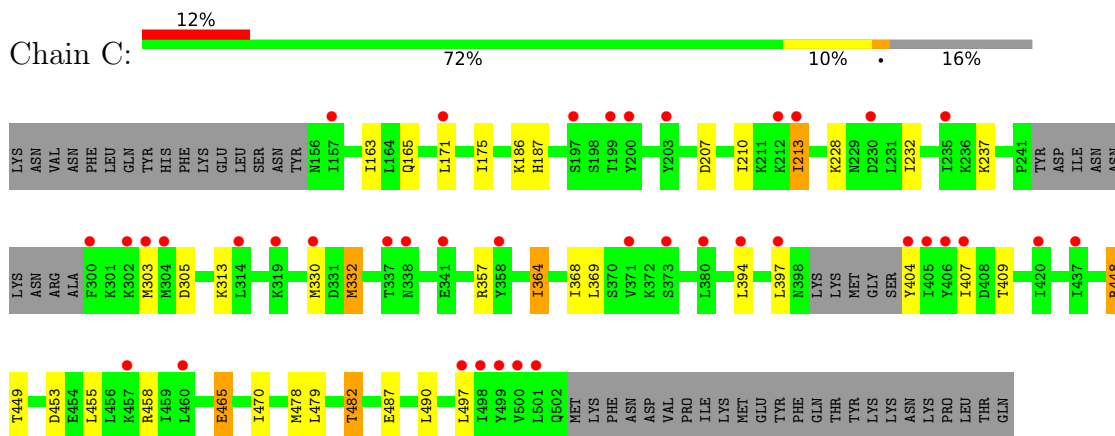
3 Residue-property plots [i](#)

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.

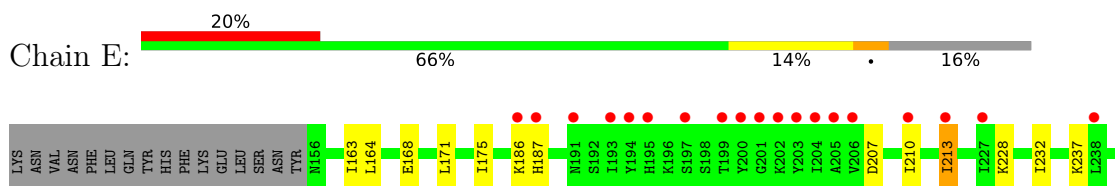
• Molecule 1: Reticulocyte-binding protein homolog 5



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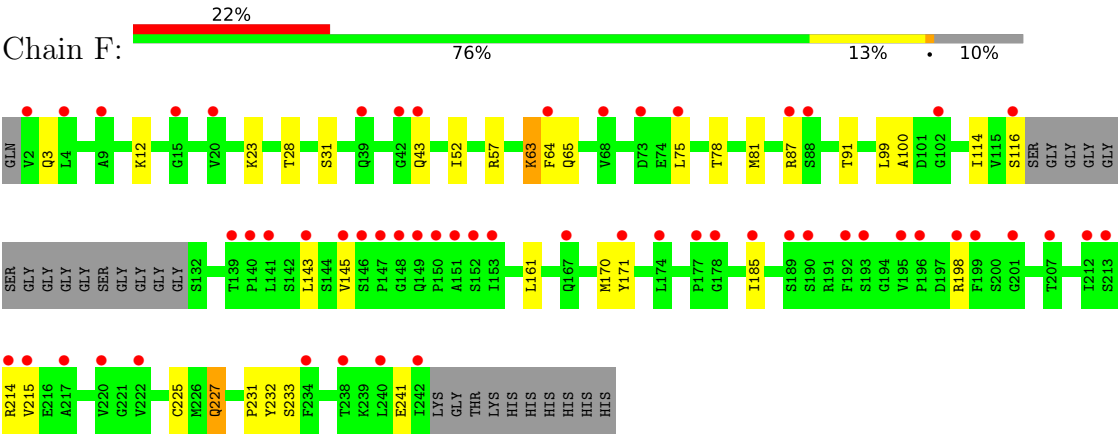


• Molecule 1: Reticulocyte-binding protein homolog 5

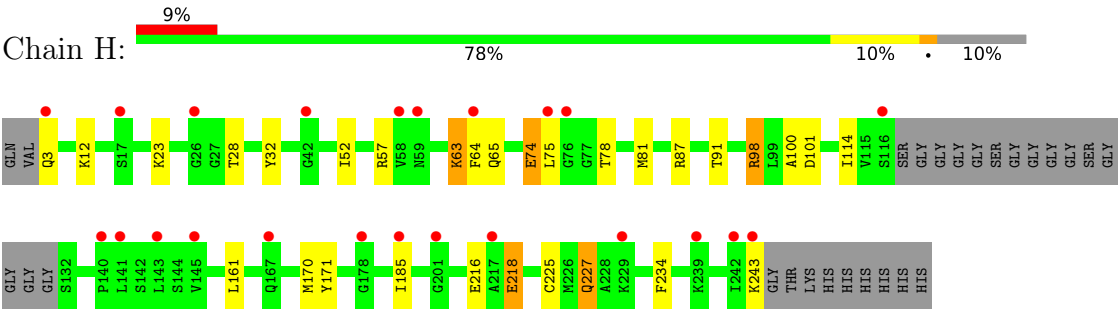


HIS
HIS

• Molecule 2: monoclonal antibody MAD8-502



• Molecule 2: monoclonal antibody MAD8-502



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.97Å 158.01Å 113.02Å 90.00° 94.59° 90.00°	Depositor
Resolution (Å)	79.00 – 2.07 79.00 – 2.07	Depositor EDS
% Data completeness (in resolution range)	96.2 (79.00-2.07) 96.2 (79.00-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.07Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-OCT-2021)	Depositor
R, R_{free}	0.269 , 0.279 0.250 , 0.258	Depositor DCC
R_{free} test set	8836 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16925	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8431e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.73	1/2464 (0.0%)	1.19	8/3307 (0.2%)
1	C	0.73	1/2464 (0.0%)	1.19	7/3307 (0.2%)
1	E	0.94	6/2455 (0.2%)	1.25	15/3295 (0.5%)
1	G	0.69	0/2440	1.17	8/3274 (0.2%)
2	B	0.71	0/1763	0.97	2/2388 (0.1%)
2	D	0.69	0/1766	0.95	0/2393
2	F	0.67	0/1757	0.92	1/2382 (0.0%)
2	H	0.68	0/1759	0.95	1/2383 (0.0%)
All	All	0.74	8/16868 (0.0%)	1.10	42/22729 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	356	ILE	CG1-CD1	6.50	1.77	1.51
1	E	438	ILE	CG1-CD1	6.32	1.76	1.51
1	C	332	MET	SD-CE	-5.81	1.65	1.79
1	E	358	TYR	N-CA	5.80	1.53	1.46
1	E	332	MET	SD-CE	-5.54	1.65	1.79
1	A	332	MET	SD-CE	-5.45	1.66	1.79
1	E	369	LEU	C-N	5.44	1.40	1.33
1	E	365	HIS	C-N	5.18	1.40	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	445	ASN	CA-CB-CG	6.89	119.49	112.60
1	E	435	THR	N-CA-C	-6.43	103.52	112.45
1	E	466	TYR	CA-C-N	6.25	128.56	120.44
1	E	466	TYR	C-N-CA	6.25	128.56	120.44
1	C	305	ASP	CA-C-N	6.22	128.62	120.28
1	C	305	ASP	C-N-CA	6.22	128.62	120.28
1	E	305	ASP	CA-C-N	6.18	128.56	120.28
1	E	305	ASP	C-N-CA	6.18	128.56	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	305	ASP	CA-C-N	6.14	128.50	120.28
1	G	305	ASP	C-N-CA	6.14	128.50	120.28
1	A	305	ASP	CA-C-N	6.07	128.42	120.28
1	A	305	ASP	C-N-CA	6.07	128.42	120.28
1	E	368	ILE	CA-C-N	5.88	128.62	120.63
1	E	368	ILE	C-N-CA	5.88	128.62	120.63
1	G	433	ASP	CA-CB-CG	5.78	118.38	112.60
1	E	371	VAL	CA-C-O	-5.76	115.06	121.17
1	G	175	ILE	CA-C-N	5.73	125.93	120.43
1	G	175	ILE	C-N-CA	5.73	125.93	120.43
1	E	175	ILE	CA-C-N	5.61	125.82	120.43
1	E	175	ILE	C-N-CA	5.61	125.82	120.43
1	A	465	GLU	CB-CG-CD	5.46	121.89	112.60
1	G	465	GLU	CB-CG-CD	5.42	121.81	112.60
1	E	369	LEU	N-CA-C	-5.41	105.02	111.03
1	C	364	ILE	N-CA-C	5.39	116.19	111.56
1	A	207	ASP	CA-CB-CG	5.38	117.97	112.60
1	G	364	ILE	N-CA-C	5.31	116.12	111.56
1	G	207	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	465	GLU	CB-CG-CD	5.28	121.57	112.60
1	E	465	GLU	CB-CG-CD	5.27	121.56	112.60
1	E	207	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	175	ILE	CA-C-N	5.18	125.40	120.43
1	A	175	ILE	C-N-CA	5.18	125.40	120.43
1	C	207	ASP	CA-CB-CG	5.17	117.77	112.60
2	B	234	PHE	CA-CB-CG	5.12	118.92	113.80
1	C	175	ILE	CA-C-N	5.11	125.34	120.43
1	C	175	ILE	C-N-CA	5.11	125.34	120.43
1	A	451	GLN	N-CA-C	-5.07	103.36	110.50
1	A	364	ILE	N-CA-C	5.06	115.91	111.56
1	E	364	ILE	N-CA-C	5.05	115.91	111.56
2	F	99	LEU	N-CA-C	5.05	117.84	109.46
2	H	234	PHE	CA-CB-CG	5.05	118.85	113.80
2	B	99	LEU	N-CA-C	5.04	117.78	109.76

There are no chirality outliers.

There are no planarity outliers.

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	2414	0	2430	17	0
1	C	2414	0	2430	19	0
1	E	2405	0	2422	32	0
1	G	2390	0	2407	23	0
2	B	1725	0	1685	19	0
2	D	1725	0	1681	12	0
2	F	1716	0	1668	16	0
2	H	1718	0	1672	17	0
3	A	43	0	0	0	0
3	B	92	0	0	0	0
3	C	69	0	0	1	0
3	D	37	0	0	0	0
3	E	102	0	0	1	0
3	F	30	0	0	0	0
3	G	10	0	0	0	0
3	H	35	0	0	0	0
All	All	16925	0	16395	145	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 4.

All (145) 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:E:356:ILE:CD1	1:E:356:ILE:CG1	1.77	1.62
1:E:438:ILE:CD1	1:E:438:ILE:CG1	1.76	1.62
2:D:227:GLN:HE21	2:D:233:SER:HB2	1.26	1.00
2:D:227:GLN:NE2	2:D:233:SER:HB2	1.79	0.96
1:G:478:MET:O	1:G:482:THR:HG23	1.78	0.84
2:F:170:MET:HE1	2:F:225:CYS:HB2	1.63	0.81
2:B:170:MET:HE1	2:B:225:CYS:HB2	1.66	0.77
2:H:161:LEU:HD22	2:H:227:GLN:HG3	1.69	0.75
2:H:170:MET:HE1	2:H:225:CYS:HB2	1.69	0.75
1:E:357:ARG:CG	1:E:446:ILE:HB	2.20	0.72
2:B:10:GLU:HG2	2:B:12:LYS:HD3	1.74	0.69
1:E:357:ARG:HG3	1:E:446:ILE:HB	1.78	0.66
2:D:136:MET:HE3	2:D:225:CYS:HB3	1.78	0.65
1:C:397:LEU:HD23	1:C:407:ILE:HG13	1.79	0.64
1:G:448:ARG:NH2	1:G:449:THR:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:454:GLU:HG3	1:G:458:ARG:HD2	1.78	0.64
1:A:351:CYS:HB3	1:A:455:LEU:HD22	1.78	0.63
1:A:237:LYS:HB3	1:A:303:MET:HE1	1.80	0.62
1:C:448:ARG:NH2	1:C:449:THR:O	2.33	0.62
2:H:161:LEU:CD2	2:H:227:GLN:HG3	2.30	0.61
1:A:448:ARG:NH1	1:A:449:THR:O	2.34	0.60
1:A:404:TYR:HB2	1:A:407:ILE:HD13	1.83	0.60
1:C:237:LYS:HB3	1:C:303:MET:HE1	1.83	0.60
1:E:237:LYS:HB3	1:E:303:MET:HE1	1.83	0.60
1:E:438:ILE:CD1	1:E:438:ILE:CB	2.76	0.59
1:G:237:LYS:HB3	1:G:303:MET:HE1	1.85	0.58
1:C:478:MET:O	1:C:482:THR:HG22	2.03	0.58
2:F:161:LEU:HD22	2:F:227:GLN:HG3	1.85	0.58
2:F:145:VAL:HG21	2:F:215:VAL:HG21	1.87	0.57
1:G:186:LYS:HG3	1:G:210:ILE:HD13	1.87	0.57
1:C:186:LYS:HG3	1:C:210:ILE:HD13	1.88	0.56
2:B:161:LEU:HD22	2:B:227:GLN:HG3	1.88	0.56
1:E:186:LYS:HG3	1:E:210:ILE:HD13	1.87	0.56
1:E:404:TYR:HB2	1:E:407:ILE:HD13	1.87	0.56
1:A:171:LEU:HD12	1:A:228:LYS:HG3	1.87	0.56
1:A:186:LYS:HG3	1:A:210:ILE:HD13	1.88	0.56
2:F:227:GLN:NE2	2:F:233:SER:OG	2.40	0.55
1:A:369:LEU:HD11	2:B:28:THR:HG21	1.88	0.55
2:B:32:TYR:CD1	2:B:98:ARG:HG3	2.42	0.54
1:G:428:THR:HG22	1:G:476:ARG:HD2	1.89	0.54
1:E:439:GLN:O	1:E:442:ILE:HG22	2.07	0.54
2:B:161:LEU:CD2	2:B:227:GLN:HG3	2.39	0.53
2:F:161:LEU:CD2	2:F:227:GLN:HG3	2.39	0.53
1:E:369:LEU:HA	1:E:372:LYS:NZ	2.23	0.52
2:F:170:MET:HE1	2:F:225:CYS:CB	2.36	0.52
2:B:161:LEU:HD22	2:B:227:GLN:CG	2.39	0.52
1:G:357:ARG:NH1	2:H:101:ASP:OD2	2.43	0.52
1:C:357:ARG:NH2	2:D:101:ASP:OD2	2.43	0.52
2:H:161:LEU:HD22	2:H:227:GLN:CG	2.38	0.52
2:D:32:TYR:CD1	2:D:98:ARG:HG3	2.46	0.51
1:C:171:LEU:HD12	1:C:228:LYS:HG3	1.93	0.51
2:B:10:GLU:CG	2:B:12:LYS:HD3	2.40	0.51
2:D:63:LYS:HZ1	2:D:132:SER:N	2.08	0.50
1:A:164:LEU:HG	1:A:478:MET:HB3	1.93	0.50
2:H:52:ILE:HD12	2:H:57:ARG:HD2	1.93	0.50
2:F:52:ILE:HD12	2:F:57:ARG:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:369:LEU:HD11	2:H:28:THR:HG21	1.94	0.50
2:H:23:LYS:HG2	2:H:78:THR:HG23	1.94	0.50
2:F:161:LEU:HD22	2:F:227:GLN:CG	2.42	0.49
2:H:74:GLU:HB3	2:H:75:LEU:HD12	1.92	0.49
1:G:165:GLN:H	1:G:482:THR:CG2	2.25	0.49
1:G:424:ILE:O	1:G:428:THR:HG23	2.12	0.49
2:B:170:MET:HE1	2:B:225:CYS:CB	2.37	0.49
1:E:241:PRO:HB3	1:E:409:THR:HG21	1.95	0.49
1:C:479:LEU:HA	1:C:482:THR:HG23	1.94	0.49
1:G:193:ILE:HD12	1:G:339:LEU:HG	1.95	0.49
1:E:419:HIS:HD2	3:E:682:HOH:O	1.97	0.48
2:H:170:MET:HE1	2:H:225:CYS:CB	2.41	0.48
1:E:369:LEU:HD11	2:F:28:THR:HG21	1.95	0.48
2:H:100:ALA:HB1	2:H:171:TYR:CE2	2.49	0.48
1:C:369:LEU:HD11	2:D:28:THR:HG21	1.96	0.47
2:D:100:ALA:HB1	2:D:171:TYR:CE2	2.49	0.47
2:B:145:VAL:HG21	2:B:215:VAL:HG21	1.96	0.46
1:E:442:ILE:HG23	1:E:443:LYS:HG3	1.97	0.46
2:F:100:ALA:HB1	2:F:171:TYR:CE2	2.50	0.46
1:E:368:ILE:HG22	1:E:372:LYS:HD3	1.96	0.46
2:B:81:MET:HE3	2:B:81:MET:HB3	1.88	0.46
2:B:231:PRO:HA	2:B:232:TYR:HA	1.79	0.46
1:E:497:LEU:O	1:E:501:LEU:HB3	2.15	0.46
1:A:397:LEU:HD23	1:A:407:ILE:HG13	1.98	0.45
2:B:100:ALA:HB1	2:B:171:TYR:CE2	2.51	0.45
2:H:81:MET:HE3	2:H:81:MET:HB3	1.91	0.45
2:B:74:GLU:O	2:B:75:LEU:HB2	2.16	0.45
1:E:368:ILE:O	1:E:372:LYS:HG3	2.17	0.45
1:E:213:ILE:HG12	1:E:332:MET:HE2	1.98	0.45
1:E:446:ILE:HD12	2:F:31:SER:HB2	1.97	0.45
1:C:237:LYS:CB	1:C:303:MET:HE1	2.46	0.45
1:E:446:ILE:HG13	1:E:447:TRP:CD1	2.52	0.45
1:G:193:ILE:HG12	1:G:202:LYS:HB2	1.98	0.45
2:H:218:GLU:H	2:H:218:GLU:HG3	1.62	0.45
1:E:237:LYS:CB	1:E:303:MET:HE1	2.45	0.45
1:G:357:ARG:HH12	2:H:101:ASP:CG	2.25	0.45
1:A:496:HIS:CE1	1:A:501:LEU:HD13	2.52	0.44
1:G:428:THR:HG22	1:G:476:ARG:CD	2.47	0.44
1:A:237:LYS:CB	1:A:303:MET:HE1	2.45	0.44
2:B:45:PRO:HD3	2:B:224:TYR:CE1	2.52	0.44
1:E:171:LEU:HB2	1:E:232:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ILE:HG12	1:C:332:MET:HE2	2.00	0.44
1:C:364:ILE:HG22	1:C:368:ILE:HD13	2.00	0.44
1:G:397:LEU:HD21	1:G:497:LEU:HD21	2.00	0.44
1:E:397:LEU:HD21	1:E:497:LEU:HD21	2.00	0.44
1:A:346:TYR:HA	1:C:313:LYS:HD3	2.01	0.43
1:C:171:LEU:HB2	1:C:232:ILE:HG12	2.00	0.43
2:H:32:TYR:CD1	2:H:98:ARG:HG3	2.54	0.43
1:G:171:LEU:HB2	1:G:232:ILE:HG12	2.00	0.43
1:A:213:ILE:HG12	1:A:332:MET:HE2	1.99	0.43
1:E:323:ASN:HD22	1:E:323:ASN:HA	1.69	0.43
1:A:171:LEU:HB2	1:A:232:ILE:HG12	2.01	0.43
1:C:404:TYR:HB3	1:C:407:ILE:HD13	2.01	0.43
1:G:237:LYS:CB	1:G:303:MET:HE1	2.48	0.42
2:D:145:VAL:HG21	2:D:215:VAL:HG21	2.01	0.42
2:H:91:THR:HG23	2:H:114:ILE:HA	2.01	0.42
1:E:442:ILE:O	1:E:446:ILE:HG23	2.19	0.42
2:D:231:PRO:HA	2:D:232:TYR:HA	1.80	0.42
2:F:231:PRO:HA	2:F:232:TYR:HA	1.81	0.42
1:E:464:ASN:O	1:E:467:SER:HB2	2.20	0.42
2:H:63:LYS:HD2	2:H:64:PHE:CZ	2.55	0.42
1:E:164:LEU:HG	1:E:478:MET:HB3	2.01	0.42
1:E:187:HIS:NE2	1:E:470:ILE:HD12	2.35	0.42
1:A:156:ASN:OD1	1:A:319:LYS:HE2	2.19	0.42
2:D:91:THR:HG23	2:D:114:ILE:HA	2.02	0.42
1:E:171:LEU:O	1:E:228:LYS:HE2	2.20	0.41
1:E:372:LYS:HB2	1:E:372:LYS:HE2	1.72	0.41
2:B:23:LYS:HG2	2:B:78:THR:HG23	2.01	0.41
2:F:91:THR:HG23	2:F:114:ILE:HA	2.02	0.41
1:C:397:LEU:HD21	1:C:497:LEU:HD21	2.02	0.41
1:C:187:HIS:NE2	1:C:470:ILE:HD12	2.35	0.41
1:E:313:LYS:HD3	1:G:346:TYR:HA	2.02	0.41
2:B:36:TRP:CE2	2:B:81:MET:HB2	2.55	0.41
2:B:91:THR:HG23	2:B:114:ILE:HA	2.02	0.41
1:G:496:HIS:CD2	1:G:500:VAL:HG21	2.56	0.41
2:B:63:LYS:HD2	2:B:64:PHE:CZ	2.55	0.41
1:G:364:ILE:HG22	1:G:368:ILE:HD13	2.03	0.41
1:E:397:LEU:HD23	1:E:407:ILE:HG13	2.02	0.41
2:F:23:LYS:HG2	2:F:78:THR:HG23	2.02	0.41
1:A:364:ILE:HG22	1:A:368:ILE:HD13	2.02	0.40
1:C:165:GLN:C	1:C:482:THR:HB	2.47	0.40
1:C:357:ARG:HD3	3:C:623:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:LYS:HD2	2:F:64:PHE:CZ	2.56	0.40
2:F:81:MET:HE3	2:F:81:MET:HB3	1.83	0.40
1:G:497:LEU:O	1:G:501:LEU:HB3	2.21	0.40
1:A:233:ALA:HA	1:A:236:LYS:HE3	2.03	0.40
1:G:187:HIS:NE2	1:G:470:ILE:HD12	2.36	0.40
1:G:397:LEU:HD23	1:G:407:ILE:HG13	2.03	0.40
2:D:45:PRO:HD3	2:D:224:TYR:CE1	2.57	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	278/338 (82%)	274 (99%)	4 (1%)	0	100	100
1	C	278/338 (82%)	275 (99%)	3 (1%)	0	100	100
1	E	277/338 (82%)	269 (97%)	8 (3%)	0	100	100
1	G	275/338 (81%)	271 (98%)	4 (2%)	0	100	100
2	B	223/252 (88%)	217 (97%)	6 (3%)	0	100	100
2	D	224/252 (89%)	219 (98%)	5 (2%)	0	100	100
2	F	223/252 (88%)	215 (96%)	8 (4%)	0	100	100
2	H	223/252 (88%)	218 (98%)	5 (2%)	0	100	100
All	All	2001/2360 (85%)	1958 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	275/327 (84%)	263 (96%)	12 (4%)	25	19
1	C	275/327 (84%)	262 (95%)	13 (5%)	23	16
1	E	274/327 (84%)	253 (92%)	21 (8%)	12	5
1	G	272/327 (83%)	257 (94%)	15 (6%)	19	12
2	B	189/202 (94%)	178 (94%)	11 (6%)	18	11
2	D	189/202 (94%)	178 (94%)	11 (6%)	18	11
2	F	188/202 (93%)	174 (93%)	14 (7%)	13	6
2	H	188/202 (93%)	176 (94%)	12 (6%)	16	9
All	All	1850/2116 (87%)	1741 (94%)	109 (6%)	18	10

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

Mol	Chain	Res	Type
1	A	163	ILE
1	A	164	LEU
1	A	213	ILE
1	A	314	LEU
1	A	330	MET
1	A	394	LEU
1	A	448	ARG
1	A	465	GLU
1	A	490	LEU
1	A	500	VAL
1	A	501	LEU
1	A	502	GLN
2	B	3	GLN
2	B	10	GLU
2	B	12	LYS
2	B	63	LYS
2	B	65	GLN
2	B	75	LEU
2	B	87	ARG
2	B	98	ARG
2	B	185	ILE
2	B	227	GLN
2	B	241	GLU

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Mol	Chain	Res	Type
1	C	163	ILE
1	C	213	ILE
1	C	330	MET
1	C	394	LEU
1	C	409	THR
1	C	448	ARG
1	C	453	ASP
1	C	455	LEU
1	C	458	ARG
1	C	465	GLU
1	C	482	THR
1	C	487	GLU
1	C	490	LEU
2	D	3	GLN
2	D	12	LYS
2	D	43	GLN
2	D	63	LYS
2	D	65	GLN
2	D	87	ARG
2	D	98	ARG
2	D	154	SER
2	D	185	ILE
2	D	233	SER
2	D	241	GLU
1	E	163	ILE
1	E	168	GLU
1	E	213	ILE
1	E	314	LEU
1	E	323	ASN
1	E	330	MET
1	E	339	LEU
1	E	343	LEU
1	E	357	ARG
1	E	368	ILE
1	E	372	LYS
1	E	443	LYS
1	E	446	ILE
1	E	451	GLN
1	E	453	ASP
1	E	455	LEU
1	E	465	GLU
1	E	487	GLU

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Mol	Chain	Res	Type
1	E	490	LEU
1	E	498	ILE
1	E	501	LEU
2	F	3	GLN
2	F	12	LYS
2	F	43	GLN
2	F	63	LYS
2	F	65	GLN
2	F	75	LEU
2	F	87	ARG
2	F	116	SER
2	F	143	LEU
2	F	185	ILE
2	F	198	ARG
2	F	214	ARG
2	F	227	GLN
2	F	241	GLU
1	G	163	ILE
1	G	193	ILE
1	G	213	ILE
1	G	228	LYS
1	G	314	LEU
1	G	330	MET
1	G	339	LEU
1	G	394	LEU
1	G	448	ARG
1	G	451	GLN
1	G	455	LEU
1	G	465	GLU
1	G	487	GLU
1	G	488	LYS
1	G	490	LEU
2	H	3	GLN
2	H	12	LYS
2	H	63	LYS
2	H	65	GLN
2	H	74	GLU
2	H	87	ARG
2	H	98	ARG
2	H	185	ILE
2	H	216	GLU
2	H	218	GLU

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Mol	Chain	Res	Type
2	H	227	GLN
2	H	243	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	338	ASN
1	A	352	ASN
1	A	398	ASN
1	A	419	HIS
1	A	495	HIS
1	C	170	HIS
1	C	338	ASN
1	C	352	ASN
1	E	156	ASN
1	E	159	ASN
1	E	338	ASN
1	E	352	ASN
1	E	354	ASN
1	E	451	GLN
1	G	170	HIS
1	G	338	ASN
1	G	502	GLN

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	284/338 (84%)	1.30	54 (19%)	3 3	55, 74, 97, 112	0
1	C	284/338 (84%)	1.14	39 (13%)	6 6	55, 67, 89, 102	0
1	E	283/338 (83%)	1.49	66 (23%)	2 1	33, 67, 98, 113	0
1	G	281/338 (83%)	1.38	58 (20%)	2 2	61, 81, 104, 117	0
2	B	227/252 (90%)	0.87	16 (7%)	22 22	50, 59, 75, 90	0
2	D	227/252 (90%)	1.14	33 (14%)	6 6	48, 70, 88, 101	1 (0%)
2	F	226/252 (89%)	1.48	56 (24%)	2 1	53, 74, 119, 155	1 (0%)
2	H	226/252 (89%)	1.05	23 (10%)	12 12	52, 66, 91, 106	1 (0%)
All	All	2038/2360 (86%)	1.24	345 (16%)	4 4	33, 70, 99, 155	3 (0%)

All (345) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	75	LEU	7.8
1	E	501	LEU	6.6
1	G	500	VAL	6.3
1	G	404	TYR	5.9
2	D	75	LEU	5.8
1	E	499	TYR	5.6
1	G	235	ILE	5.5
2	B	75	LEU	5.5
1	E	404	TYR	5.4
1	E	498	ILE	5.4
1	C	499	TYR	5.4
1	E	500	VAL	5.3
1	A	404	TYR	5.0
1	A	499	TYR	5.0
1	E	200	TYR	5.0
2	F	242	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	203	TYR	4.9
1	C	500	VAL	4.7
1	A	302	LYS	4.6
1	E	405	ILE	4.6
1	C	404	TYR	4.5
2	F	217	ALA	4.4
2	H	243	LYS	4.3
1	A	405	ILE	4.3
2	F	147	PRO	4.3
1	C	300	PHE	4.2
1	E	497	LEU	4.1
1	A	500	VAL	4.1
1	A	241	PRO	4.1
1	G	300	PHE	4.1
2	H	75	LEU	4.1
1	E	406	TYR	4.1
1	A	300	PHE	4.0
1	C	405	ILE	4.0
1	G	397	LEU	4.0
1	G	499	TYR	4.0
1	A	157	ILE	3.9
2	F	212	ILE	3.9
1	G	338	ASN	3.9
1	G	405	ILE	3.9
2	F	2	VAL	3.9
2	F	150	PRO	3.9
1	G	193	ILE	3.8
2	F	215	VAL	3.8
2	D	63	LYS	3.8
2	H	242	ILE	3.7
1	C	373	SER	3.7
2	F	73	ASP	3.7
1	E	199	THR	3.7
1	G	309	THR	3.7
1	E	336	GLY	3.6
2	F	88	SER	3.6
1	E	300	PHE	3.6
2	F	141	LEU	3.6
2	D	2	VAL	3.6
2	B	2	VAL	3.5
1	G	393	LEU	3.5
2	H	116	SER	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	42	GLY	3.5
2	H	141	LEU	3.5
2	F	116	SER	3.4
2	H	76	GLY	3.4
1	A	406	TYR	3.4
1	G	501	LEU	3.4
1	E	323	ASN	3.3
1	E	409	THR	3.3
1	G	163	ILE	3.3
1	E	303	MET	3.3
2	D	217	ALA	3.3
2	F	167	GLN	3.2
1	E	344	SER	3.2
2	F	42	GLY	3.2
1	C	437	ILE	3.2
1	E	346	TYR	3.2
1	E	350	PHE	3.2
1	E	390	SER	3.2
1	G	302	LYS	3.2
1	E	393	LEU	3.2
1	E	407	ILE	3.2
1	G	498	ILE	3.2
2	F	143	LEU	3.2
1	G	428	THR	3.2
2	F	148	GLY	3.2
1	C	157	ILE	3.1
1	E	197	SER	3.1
1	A	199	THR	3.1
2	F	201	GLY	3.1
1	E	394	LEU	3.1
1	A	232	ILE	3.1
1	A	303	MET	3.1
1	C	200	TYR	3.1
1	G	177	PRO	3.1
2	F	213	SER	3.1
1	C	338	ASN	3.0
2	D	243	LYS	3.0
1	E	392	LEU	3.0
1	E	373	SER	3.0
1	E	194	TYR	3.0
2	F	64	PHE	3.0
1	C	497	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	206	VAL	3.0
1	G	341	GLU	3.0
1	G	213	ILE	3.0
1	E	186	LYS	3.0
1	C	303	MET	3.0
1	E	238	LEU	2.9
1	C	235	ILE	2.9
1	G	406	TYR	2.9
1	C	397	LEU	2.9
1	C	498	ILE	2.9
1	A	393	LEU	2.9
1	G	315	ILE	2.9
2	D	116	SER	2.9
1	G	320	ASN	2.9
2	F	174	LEU	2.8
1	A	398	ASN	2.8
2	D	238	THR	2.8
2	F	220	VAL	2.8
1	A	319	LYS	2.8
2	H	42	GLY	2.8
1	A	394	LEU	2.8
1	C	337	THR	2.8
1	G	167	LYS	2.8
1	G	319	LYS	2.8
1	G	172	ASP	2.7
1	E	201	GLY	2.7
1	C	406	TYR	2.7
1	E	343	LEU	2.7
1	A	156	ASN	2.7
1	E	187	HIS	2.7
2	F	152[A]	SER	2.7
1	G	158	ALA	2.7
1	E	338	ASN	2.7
2	H	58	VAL	2.7
1	G	407	ILE	2.7
2	B	132	SER	2.7
1	E	340	PHE	2.7
1	E	397	LEU	2.7
1	G	482	THR	2.7
2	F	238	THR	2.7
1	E	241	PRO	2.7
2	D	132	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	163	ILE	2.7
2	F	151	ALA	2.6
1	A	171	LEU	2.6
1	A	197	SER	2.6
2	F	189	SER	2.6
1	A	437	ILE	2.6
2	D	145	VAL	2.6
2	H	167	GLN	2.6
1	A	323	ASN	2.6
1	A	339	LEU	2.6
1	E	314	LEU	2.6
1	A	301	LYS	2.6
2	F	190	SER	2.6
1	E	358	TYR	2.6
1	G	480	TYR	2.6
2	B	87	ARG	2.6
1	C	407	ILE	2.6
2	H	201	GLY	2.6
2	D	228	ALA	2.6
1	A	380	LEU	2.6
1	C	501	LEU	2.6
2	B	66	GLY	2.6
2	D	26	GLY	2.6
1	G	330	MET	2.6
1	A	309	THR	2.6
1	C	314	LEU	2.6
2	D	85	SER	2.6
2	F	240	LEU	2.6
2	D	167	GLN	2.5
1	C	304	MET	2.5
2	D	225	CYS	2.5
1	C	302	LYS	2.5
1	C	457	LYS	2.5
2	H	229	LYS	2.5
2	F	207	THR	2.5
2	F	146	SER	2.5
1	A	213	ILE	2.5
1	E	204	ILE	2.5
2	F	198	ARG	2.5
1	A	409	THR	2.5
1	A	344	SER	2.5
1	G	241	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	88	SER	2.5
2	H	143	LEU	2.5
1	A	412	PHE	2.5
1	E	302	LYS	2.5
2	F	20	VAL	2.5
2	F	4	LEU	2.5
1	G	303	MET	2.5
2	F	199	PHE	2.5
1	A	484	TYR	2.4
1	C	330	MET	2.4
1	A	501	LEU	2.4
1	G	171	LEU	2.4
1	A	227	ILE	2.4
1	C	199	THR	2.4
2	D	28	THR	2.4
2	D	139	THR	2.4
2	F	140	PRO	2.4
2	D	174	LEU	2.4
1	A	304	MET	2.4
1	E	466	TYR	2.4
1	A	195	HIS	2.4
1	A	392	LEU	2.4
1	E	339	LEU	2.4
1	C	230	ASP	2.4
1	G	420	ILE	2.4
2	F	185	ILE	2.4
1	G	199	THR	2.4
1	G	217	TYR	2.3
2	D	187	GLU	2.3
1	G	376	LEU	2.3
2	H	59	ASN	2.3
2	B	64	PHE	2.3
2	H	17	SER	2.3
2	H	185	ILE	2.3
2	H	140	PRO	2.3
1	E	307	TYR	2.3
2	D	59	ASN	2.3
1	C	171	LEU	2.3
1	G	169	GLY	2.3
2	H	178	GLY	2.3
1	A	236	LYS	2.3
2	F	192	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	213	ILE	2.3
1	C	420	ILE	2.3
1	E	193	ILE	2.3
1	G	161	ILE	2.3
1	A	502	GLN	2.3
2	F	43	GLN	2.3
2	D	9	ALA	2.3
2	D	76	GLY	2.3
1	G	178	HIS	2.3
2	B	25	SER	2.3
2	D	25	SER	2.3
1	G	220	VAL	2.3
2	F	68	VAL	2.3
2	H	145	VAL	2.3
1	E	372	LYS	2.3
2	F	178	GLY	2.3
1	A	497	LEU	2.3
1	E	480	TYR	2.3
1	G	307	TYR	2.3
2	B	80	TYR	2.3
1	C	197	SER	2.2
2	D	64	PHE	2.2
1	A	410	ILE	2.2
1	E	213	ILE	2.2
2	D	68	VAL	2.2
2	D	147	PRO	2.2
2	F	87	ARG	2.2
1	E	304	MET	2.2
2	F	15	GLY	2.2
1	A	468	LEU	2.2
1	C	394	LEU	2.2
2	D	143	LEU	2.2
1	C	358	TYR	2.2
1	E	195	HIS	2.2
2	F	153	ILE	2.2
2	F	177	PRO	2.2
2	H	239	LYS	2.2
2	D	42	GLY	2.2
1	G	314	LEU	2.2
1	G	339	LEU	2.2
2	B	43	GLN	2.2
2	D	193	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	212	LYS	2.2
1	E	347	ASN	2.2
1	E	210	ILE	2.2
1	E	309	THR	2.2
2	F	196	PRO	2.2
2	F	102	GLY	2.2
1	E	205	ALA	2.2
1	A	419	HIS	2.2
2	F	149	GLN	2.2
1	A	479	LEU	2.2
1	C	460	LEU	2.2
1	A	390	SER	2.2
2	F	193	SER	2.2
1	A	186	LYS	2.2
2	D	81	MET	2.2
2	F	139	THR	2.2
1	C	341	GLU	2.1
1	E	413	ILE	2.1
1	G	318	ILE	2.1
2	F	234	PHE	2.1
1	C	371	VAL	2.1
2	B	68	VAL	2.1
2	F	222	VAL	2.1
2	B	194	GLY	2.1
1	A	198	SER	2.1
1	C	319	LYS	2.1
1	E	398	ASN	2.1
1	G	323	ASN	2.1
2	B	133	ASN	2.1
2	F	39	GLN	2.1
1	A	350	PHE	2.1
2	H	64	PHE	2.1
2	B	26	GLY	2.1
2	B	76	GLY	2.1
2	F	145	VAL	2.1
1	G	476	ARG	2.1
2	F	9	ALA	2.1
2	H	217	ALA	2.1
1	A	164	LEU	2.1
1	E	202	LYS	2.1
1	E	301	LYS	2.1
1	G	453	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	363	TYR	2.1
2	F	171	TYR	2.1
1	G	342	GLN	2.1
1	E	469	PHE	2.1
2	F	195	VAL	2.1
1	A	167	LYS	2.1
1	G	212	LYS	2.1
1	C	380	LEU	2.1
1	E	455	LEU	2.1
1	G	160	SER	2.1
1	G	198	SER	2.1
2	B	236	GLN	2.1
2	D	149	GLN	2.1
1	A	384	THR	2.1
2	H	26	GLY	2.1
1	E	227	ILE	2.1
1	E	356	ILE	2.1
1	E	431	ILE	2.1
1	E	442	ILE	2.1
2	D	70	ILE	2.1
1	G	304	MET	2.0
1	G	387	LEU	2.0
1	C	203	TYR	2.0
2	D	194	GLY	2.0
1	A	413	ILE	2.0
1	A	498	ILE	2.0
1	A	341	GLU	2.0
1	E	191	ASN	2.0
1	G	164	LEU	2.0
2	H	3	GLN	2.0
2	F	214	ARG	2.0
1	G	419	HIS	2.0
1	G	474	HIS	2.0
1	A	411	LYS	2.0
1	E	395	THR	2.0

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

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.