



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:28 PM UTC

PDB ID : 6RYA / pdb_00006rya
Title : Structure of Dup1 mutant H67A:Ubiquitin complex
Authors : Donghyuk, S.; Ivan, D.
Deposited on : 2019-06-10
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

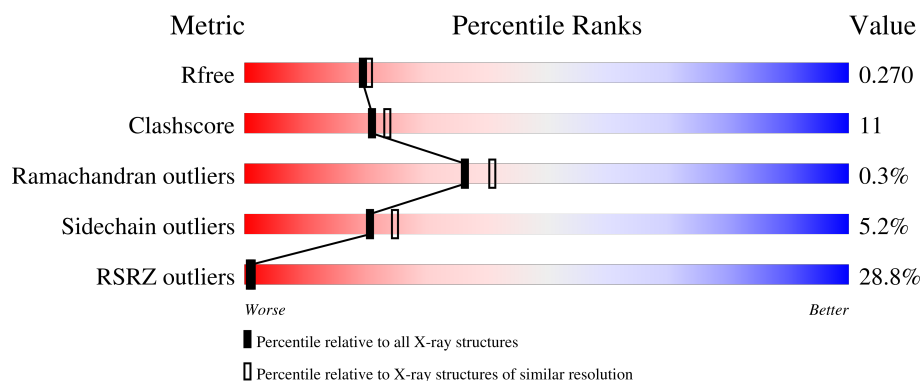
1 Overall quality at a glance

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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	343	26% 71% 17% 10%
1	C	343	28% 60% 27% 10%
1	E	343	25% 71% 17% 10%
2	B	76	33% 72% 24% •
2	D	76	13% 79% 18% •

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Mol	Chain	Length	Quality of chain
2	F	76	36% 84% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9240 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 Septation initiation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2472	1569	435	459	9			
1	C	308	Total	C	N	O	S	0	0	0
			2472	1569	435	459	9			
1	E	308	Total	C	N	O	S	0	0	0
			2472	1569	435	459	9			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	-	expression tag	UNP A0A3A6VНК6
A	67	ALA	HIS	conflict	UNP A0A3A6VНК6
A	228	ASP	ALA	conflict	UNP A0A3A6VНК6
C	3	SER	-	expression tag	UNP A0A3A6VНК6
C	67	ALA	HIS	conflict	UNP A0A3A6VНК6
C	228	ASP	ALA	conflict	UNP A0A3A6VНК6
E	3	SER	-	expression tag	UNP A0A3A6VНК6
E	67	ALA	HIS	conflict	UNP A0A3A6VНК6
E	228	ASP	ALA	conflict	UNP A0A3A6VНК6

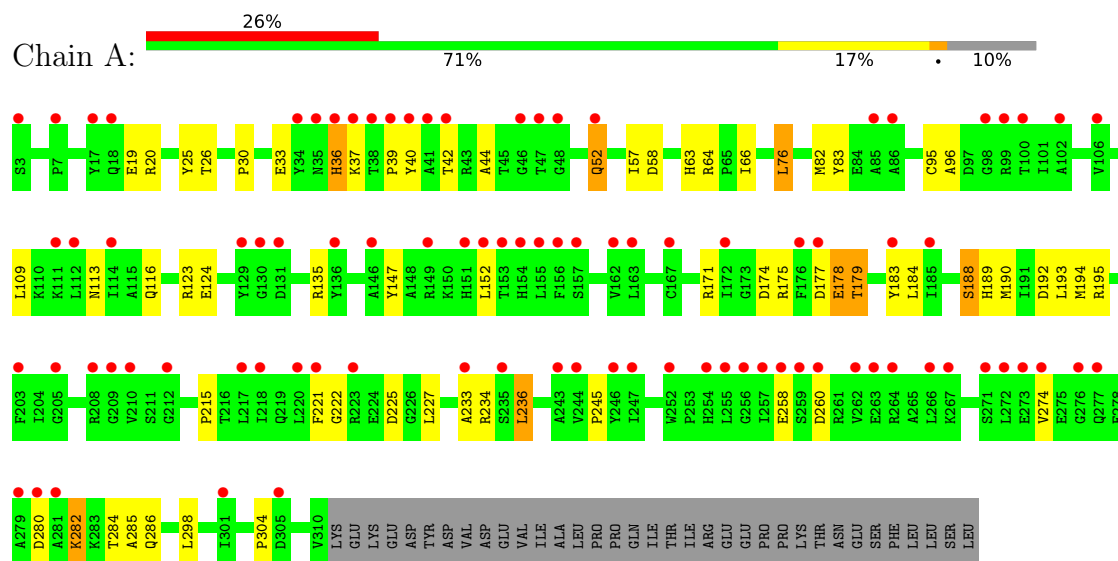
- Molecule 2 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	1	0
			608	383	106	118	1			
2	D	76	Total	C	N	O	S	0	1	0
			608	383	106	118	1			
2	F	76	Total	C	N	O	S	0	1	0
			608	383	106	118	1			

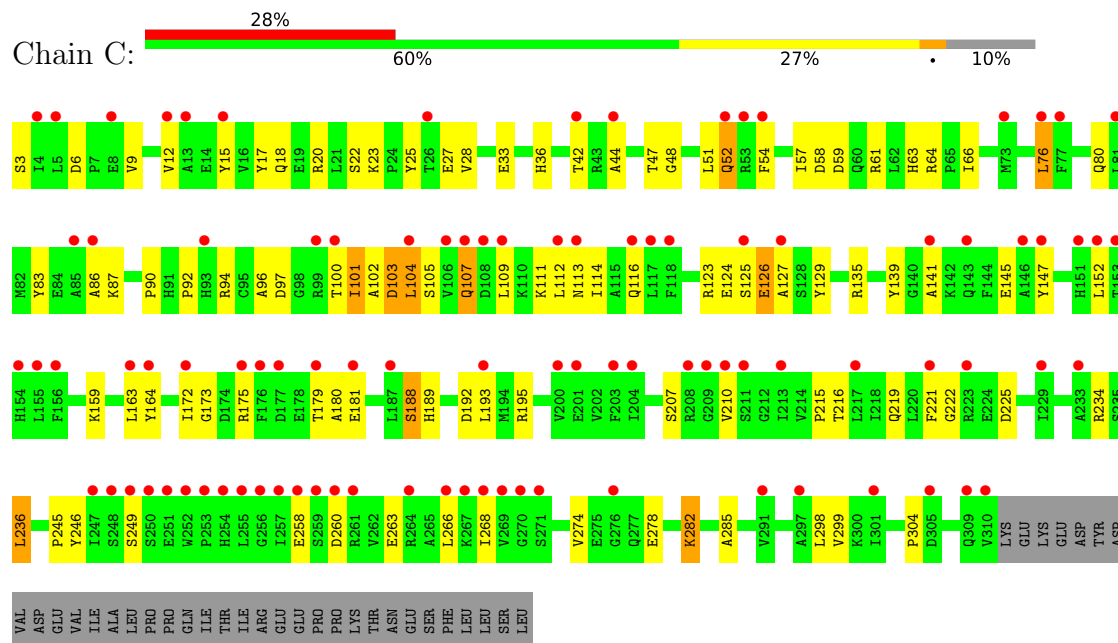
3 Residue-property plots [i](#)

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: Septation initiation protein



• Molecule 1: Septation initiation protein



Chain E:

25% 71% 17% 10%

Label	Color
L286	Red
K267	Red
I268	Red
S3	Red
I4	Red
S771	Red
L272	Red
E273	Red
V274	Red
K282	Red
Q286	Red
V291	Red
C294	Red
L288	Red
V299	Red
D302	Red
V310	Red
LYS	Red
GLY	Red
LYS	Red
LYS	Red
GLU	Red
ASP	Red
TYR	Red
ASP	Red
VAL	Red
ASP	Red
GLU	Red
VAL	Red
ILE	Red
ALA	Red
LEU	Red
PRO	Red
PRO	Red
GLN	Red
ILE	Red
THR	Red
ILE	Red
ARG	Red
GLU	Red
GLU	Red
PRO	Red
PRO	Red
LYS	Red
THR	Red
ASN	Red
GLU	Red
SER	Red
PHE	Red
LEU	Red
LEU	Red
SER	Red
LEU	Red
L286	Red
K267	Red
I268	Red
S3	Red
I4	Red
S771	Red
L272	Red
E273	Red
V274	Red
K282	Red
Q286	Red
V291	Red
C294	Red
L288	Red
V299	Red
D302	Red
V310	Red
LYS	Red
GLY	Red
LYS	Red
LYS	Red
GLU	Red
ASP	Red
TYR	Red
ASP	Red
VAL	Red
ASP	Red
GLU	Red
VAL	Red
ILE	Red
ALA	Red
LEU	Red
PRO	Red
PRO	Red
GLN	Red
ILE	Red
THR	Red
ILE	Red
ARG	Red
GLU	Red
GLU	Red
PRO	Red
PRO	Red
LYS	Red
THR	Red
ASN	Red
GLU	Red
SER	Red
PHE	Red
LEU	Red
LEU	Red
SER	Red
LEU	Red
L286	Red
K267	Red
I268	Red
S3	Red
I4	Red
S771	Red
L272	Red
E273	Red
V274	Red
K282	Red
Q286	Red
V291	Red
C294	Red
L288	Red
V299	Red
D302	Red
V310	Red
LYS	Red
GLY	Red
LYS	Red
LYS	Red
GLU	Red
ASP	Red
TYR	Red
ASP	Red
VAL	Red
ASP	Red
GLU	Red
VAL	Red
ILE	Red
ALA	Red
LEU	Red
PRO	Red
PRO	Red
GLN	Red
ILE	Red
THR	Red
ILE	Red
ARG	Red
GLU	Red
GLU	Red
PRO	Red
PRO	Red
LYS	Red
THR	Red
ASN	Red
GLU	Red
SER	Red
PHE	Red
LEU	Red
LEU	Red
SER	Red
LEU	Red
L286	Red
K267	Red
I268	Red
S3	Red
I4	Red
S771	Red
L272	Red
E273	Red
V274	Red
K282	Red
Q286	Red
V291	Red
C294	Red
L288	Red
V299	Red
D302	Red
V310	Red
LYS	Red
GLY	Red
LYS	Red
LYS	Red
GLU	Red
ASP	Red
TYR	Red
ASP	Red
VAL	Red
ASP	Red
GLU	Red
VAL	Red
ILE	Red
ALA	Red
LEU	Red
PRO	Red
PRO	Red
GLN	Red
ILE	Red
THR	Red
ILE	Red
ARG	Red
GLU	Red
GLU	Red
PRO	Red
PRO	Red
LYS	Red
THR	Red
ASN	Red
GLU	Red
SER	Red
PHE	Red
LEU	Red
LEU	Red
SER	Red
LEU	Red
L286	Red
K267	Red
I268	Red
S3	Red
I4	Red
S771	Red
L272	Red
E273	Red
V274	Red
K282	Red
Q286	Red
V291	Red
C294	Red
L288	Red
V299	Red
D302	Red
V310	Red
LYS	Red
GLY	Red
LYS	Red
LYS	Red
GLU	Red
ASP	Red
TYR	Red
ASP	

Chain B:

33%

72%

24%

Chain D:

Bar Label	Color	Red Dot
M1	Orange	No
Q2	Green	Yes
V5	Green	No
K6	Yellow	Yes
T7	Green	No
L8	Yellow	No
T9	Green	Yes
G10	Green	No
K11	Yellow	Yes
T12	Green	Yes
T13	Green	Yes
L15	Green	No
E16	Green	No
V17	Green	Yes
E18	Green	No
P19	Green	Yes
I30	Yellow	No
E34	Yellow	No
P38	Green	No
D39	Orange	No
Q40	Green	No
E51	Yellow	No
R54	Yellow	No
T55	Yellow	Yes
S65	Green	Yes
V70	Green	No
L71	Green	No
R72	Green	No
L73	Green	No
R74	Yellow	No
G75	Green	No
G76	Green	No

Chain F:

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.33Å 67.14Å 182.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 2.21 49.07 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.07-2.21) 99.7 (49.07-2.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.209 , 0.289 (Not available) , 0.270	Depositor DCC
R_{free} test set	3463 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.108 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.115 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.058 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.057 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.046 for -h,-k,l	Xtriage
Reported twinning fraction	0.176 for H, K, L 0.169 for h,-k,-l 0.162 for -1/2H-3/2K, -1/2H+1/2K, -L 0.167 for -1/2H+3/2K, 1/2H+1/2K, -L 0.159 for 1/2H-3/2K, -1/2H-1/2K, -L 0.167 for 1/2H+3/2K, 1/2H-1/2K, -L	Depositor
Outliers	0 of 71216 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9240	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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	1.16	1/2534 (0.0%)	1.55	3/3430 (0.1%)
1	C	1.16	2/2534 (0.1%)	1.54	5/3430 (0.1%)
1	E	1.16	3/2534 (0.1%)	1.55	7/3430 (0.2%)
2	B	1.19	1/617 (0.2%)	1.54	3/827 (0.4%)
2	D	1.15	0/617	1.51	0/827
2	F	1.19	0/617	1.57	4/827 (0.5%)
All	All	1.16	7/9453 (0.1%)	1.55	22/12771 (0.2%)

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	C	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	THR	C-O	6.83	1.32	1.23
1	E	179	THR	C-O	6.08	1.31	1.23
1	C	189	HIS	CE1-NE2	5.40	1.38	1.32
2	B	36	ILE	N-CA	5.30	1.50	1.46
1	E	25	TYR	C-O	5.18	1.30	1.24
1	C	278	GLU	C-O	5.09	1.30	1.23
1	E	65	PRO	C-O	-5.02	1.18	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	GLY	CA-C-O	-7.55	116.18	122.29
1	C	222	GLY	CA-C-O	-6.64	116.91	122.29
1	E	222	GLY	CA-C-O	-6.48	116.61	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	167	CYS	CB-CA-C	-6.40	100.74	110.92
1	C	58	ASP	CA-CB-CG	6.32	118.92	112.60
1	C	189	HIS	CA-C-N	6.07	128.33	120.44
1	C	189	HIS	C-N-CA	6.07	128.33	120.44
1	E	302	ASP	CA-CB-CG	5.70	118.30	112.60
2	B	36	ILE	CA-C-N	5.67	123.80	119.66
2	B	36	ILE	C-N-CA	5.67	123.80	119.66
1	C	188	SER	CA-C-O	-5.65	115.08	120.90
1	A	189	HIS	CA-C-N	5.58	127.69	120.44
1	A	189	HIS	C-N-CA	5.58	127.69	120.44
1	E	22	SER	O-C-N	5.41	127.64	122.07
1	E	189	HIS	CA-C-N	5.35	127.40	120.44
1	E	189	HIS	C-N-CA	5.35	127.40	120.44
1	E	103	ASP	CA-CB-CG	5.26	117.86	112.60
2	F	51	GLU	CA-C-N	5.18	127.64	120.29
2	F	51	GLU	C-N-CA	5.18	127.64	120.29
2	F	37	PRO	N-CA-CB	5.14	106.07	103.19
2	B	70	VAL	CA-C-O	-5.11	114.81	120.74
2	F	46	ALA	CA-C-O	-5.01	114.42	119.78

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	173	GLY	Peptide
1	C	188	SER	Mainchain

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	2472	0	2405	58	0
1	C	2472	0	2405	81	17
1	E	2472	0	2405	38	0
2	B	608	0	642	16	0
2	D	608	0	642	17	0
2	F	608	0	642	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9240	0	9141	202	17

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 11.

All (202) 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:96:ALA:HB2	1:A:175:ARG:NH2	1.50	1.24
1:C:101:ILE:HD11	1:C:180:ALA:O	1.39	1.21
1:C:100:THR:OG1	1:C:103:ASP:OD2	1.61	1.16
1:A:96:ALA:CB	1:A:175:ARG:HH21	1.59	1.13
1:C:27:GLU:HB2	1:C:125:SER:HB3	1.22	1.13
1:A:96:ALA:HB2	1:A:175:ARG:HH21	0.89	1.02
1:C:27:GLU:CB	1:C:125:SER:HB3	2.01	0.89
1:A:177:ASP:HB3	1:A:183:TYR:CD1	2.10	0.86
2:B:8:LEU:HD11	2:B:70:VAL:HG22	1.58	0.86
2:F:8:LEU:HD11	2:F:70:VAL:HG22	1.56	0.85
1:A:96:ALA:CB	1:A:175:ARG:NH2	2.29	0.83
1:C:47:THR:HG21	2:D:51:GLU:HG2	1.64	0.76
1:C:51:LEU:O	1:C:126:GLU:HG3	1.88	0.73
1:E:224:GLU:CG	1:E:225:ASP:H	2.00	0.73
1:E:224:GLU:HG2	1:E:225:ASP:H	1.54	0.72
1:A:194:MET:HE1	1:A:233:ALA:HB3	1.70	0.72
1:A:171:ARG:HB3	1:A:174:ASP:OD1	1.91	0.70
1:C:27:GLU:HG3	1:C:124:GLU:HB3	1.73	0.70
1:C:101:ILE:HA	1:C:104:LEU:HG	1.75	0.69
2:D:8:LEU:HD11	2:D:70:VAL:HG22	1.76	0.68
1:C:83:TYR:O	1:C:87:LYS:HG3	1.94	0.68
2:B:21:ASP:OD1	2:B:25:ASN:HB3	1.93	0.67
1:A:52:GLN:CD	2:B:40:GLN:HE22	2.02	0.67
1:E:234:ARG:NH1	1:E:245:PRO:O	2.27	0.66
1:C:20:ARG:NH2	1:C:124:GLU:OE2	2.28	0.66
1:C:92:PRO:HG3	1:C:102:ALA:HB2	1.78	0.65
1:C:92:PRO:HG3	1:C:102:ALA:CB	2.25	0.65
1:C:51:LEU:O	1:C:126:GLU:CG	2.44	0.65
1:C:27:GLU:HB2	1:C:125:SER:CB	2.13	0.65
1:A:36:HIS:ND1	1:A:37:LYS:N	2.46	0.64
1:A:177:ASP:O	1:A:179:THR:N	2.31	0.64
1:A:234:ARG:NH1	1:A:245:PRO:O	2.30	0.63
1:C:234:ARG:NH1	1:C:245:PRO:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:LEU:HD13	1:C:298:LEU:HD22	1.80	0.62
1:C:48:GLY:O	1:C:126:GLU:C	2.45	0.60
1:A:96:ALA:CA	1:A:175:ARG:NH2	2.64	0.60
1:A:95:CYS:SG	1:A:177:ASP:HB2	2.42	0.60
1:E:3:SER:O	1:E:299:VAL:HG12	2.02	0.59
1:A:40:TYR:CZ	2:D:74:ARG:HG2	2.39	0.58
2:D:6:LYS:HG2	2:D:12:THR:HG23	1.86	0.57
1:C:219:GLN:NE2	1:C:268:ILE:HD13	2.18	0.57
1:C:3:SER:O	1:C:299:VAL:HG12	2.05	0.57
1:C:141:ALA:O	1:C:145:GLU:HG3	2.04	0.57
1:E:208:ARG:HG3	1:E:261:ARG:HD3	1.87	0.56
1:C:101:ILE:HD12	1:C:180:ALA:HB1	1.87	0.56
1:A:284:THR:HG23	2:B:72:ARG:NH1	2.21	0.56
1:C:103:ASP:OD2	1:C:103:ASP:N	2.39	0.56
1:A:96:ALA:HB2	1:A:175:ARG:CZ	2.30	0.56
1:A:40:TYR:OH	2:D:74:ARG:NE	2.38	0.55
1:A:96:ALA:N	1:A:175:ARG:NH2	2.53	0.55
1:C:107:GLN:NE2	1:C:111:LYS:NZ	2.54	0.55
1:C:163:LEU:HD11	1:C:179:THR:HG21	1.87	0.55
1:E:20:ARG:NH2	1:E:124:GLU:OE2	2.39	0.55
2:B:36:ILE:HG22	2:B:41:GLN:HE21	1.72	0.55
2:B:45:PHE:HB3	2:B:50:LEU:HD21	1.88	0.55
1:C:48:GLY:O	1:C:126:GLU:HB3	2.06	0.55
2:B:6:LYS:HG2	2:B:12:THR:HG23	1.88	0.54
1:C:107:GLN:NE2	1:C:111:LYS:CE	2.70	0.54
1:C:107:GLN:NE2	1:C:111:LYS:HE3	2.23	0.54
1:C:101:ILE:CD1	1:C:180:ALA:HB1	2.38	0.54
1:C:135:ARG:HG2	1:C:139:TYR:CZ	2.42	0.53
1:A:96:ALA:N	1:A:175:ARG:HH22	2.06	0.53
2:D:72:ARG:O	2:D:72:ARG:NH2	2.40	0.53
1:E:147:TYR:HE1	1:E:152:LEU:HD11	1.73	0.53
1:C:192:ASP:O	1:C:195:ARG:NH1	2.41	0.53
1:C:48:GLY:O	1:C:126:GLU:O	2.28	0.52
1:A:20:ARG:NH2	1:A:124:GLU:OE2	2.42	0.52
1:E:56:THR:HG22	1:E:59:ASP:HA	1.92	0.52
1:C:6:ASP:HB3	1:C:9:VAL:HG23	1.90	0.52
1:C:76:LEU:CD2	1:C:116:GLN:HB2	2.40	0.52
1:C:107:GLN:O	1:C:111:LYS:NZ	2.33	0.52
1:A:57:ILE:HG21	1:A:285:ALA:HB2	1.92	0.51
2:F:1:MET:N	2:F:17:VAL:O	2.40	0.51
1:C:18:GLN:O	1:C:23:LYS:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:HIS:O	1:A:39:PRO:HD3	2.11	0.51
1:E:8:GLU:OE2	1:E:154:HIS:NE2	2.42	0.51
1:E:101:ILE:HD11	1:E:183:TYR:CE2	2.46	0.51
1:E:221:PHE:O	1:E:225:ASP:HB2	2.10	0.51
2:B:34:GLU:OE1	2:B:74:ARG:NH2	2.44	0.50
1:C:27:GLU:O	1:C:125:SER:HB2	2.11	0.50
2:F:6:LYS:HG2	2:F:12:THR:HG23	1.92	0.50
1:C:17:TYR:O	1:C:22:SER:OG	2.25	0.50
1:A:221:PHE:O	1:A:225:ASP:HB2	2.11	0.50
1:E:56:THR:CG2	1:E:59:ASP:HA	2.42	0.50
1:A:63:HIS:O	1:A:64:ARG:C	2.54	0.49
1:C:96:ALA:HB2	1:C:175:ARG:NH2	2.28	0.49
1:E:96:ALA:HB2	1:E:175:ARG:NH2	2.28	0.49
1:E:76:LEU:CD2	1:E:116:GLN:HB2	2.42	0.49
1:E:80:GLN:OE1	1:E:109:LEU:CD2	2.61	0.48
2:D:34:GLU:OE1	2:D:74:ARG:NH2	2.46	0.48
1:A:147:TYR:HE1	1:A:152:LEU:HD11	1.78	0.48
1:E:55:ILE:HD12	1:E:57:ILE:HD11	1.94	0.48
1:C:76:LEU:HD13	1:C:113:ASN:HB3	1.96	0.48
1:C:80:GLN:NE2	1:C:109:LEU:HG	2.29	0.47
2:D:39:ASP:OD1	2:D:39:ASP:C	2.57	0.47
1:E:52:GLN:OE1	2:F:40:GLN:OE1	2.32	0.47
1:C:147:TYR:HE1	1:C:152:LEU:HD11	1.79	0.47
1:E:80:GLN:OE1	1:E:109:LEU:HD23	2.13	0.47
1:A:236:LEU:HD13	1:A:298:LEU:HD22	1.96	0.47
2:B:1:MET:N	2:B:17:VAL:O	2.45	0.47
1:E:224:GLU:CG	1:E:225:ASP:N	2.69	0.47
1:C:33:GLU:O	1:C:42:THR:HG21	2.15	0.47
1:E:33:GLU:O	1:E:42:THR:HG21	2.14	0.47
1:A:30:PRO:HA	1:A:33:GLU:CD	2.40	0.46
1:E:76:LEU:CD2	1:E:116:GLN:CB	2.93	0.46
1:A:36:HIS:ND1	1:A:36:HIS:C	2.71	0.46
2:D:1:MET:N	2:D:17:VAL:O	2.45	0.46
1:C:76:LEU:CD2	1:C:116:GLN:CB	2.93	0.46
1:E:109:LEU:HD12	1:E:112:LEU:HD22	1.96	0.46
1:A:52:GLN:HE21	2:B:72:ARG:HB2	1.81	0.46
1:C:54:PHE:CD2	1:C:61:ARG:HG2	2.51	0.46
1:C:101:ILE:HD11	1:C:180:ALA:C	2.30	0.46
1:E:25:TYR:CZ	1:E:64:ARG:HB3	2.51	0.46
1:C:27:GLU:C	1:C:28:VAL:HG13	2.39	0.46
1:C:52:GLN:HG3	1:C:66:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ARG:NH2	1:C:123:ARG:O	2.49	0.46
1:C:258:GLU:N	1:C:258:GLU:OE2	2.48	0.46
1:E:236:LEU:HD13	1:E:298:LEU:HD22	1.98	0.46
2:B:21:ASP:OD1	2:B:25:ASN:CB	2.62	0.45
1:A:64:ARG:NH2	1:A:123:ARG:O	2.50	0.45
1:C:112:LEU:HA	1:C:164:TYR:CE1	2.52	0.45
1:E:147:TYR:CE1	1:E:152:LEU:HD11	2.51	0.45
2:B:72:ARG:O	2:B:72:ARG:NH2	2.47	0.45
1:C:36:HIS:CD2	2:D:54:ARG:NH1	2.85	0.45
1:E:97:ASP:OD2	1:E:99:ARG:NH1	2.49	0.45
1:A:33:GLU:O	1:A:42:THR:HG21	2.16	0.44
1:E:70:ALA:O	1:E:74:ARG:HG3	2.16	0.44
1:E:224:GLU:HG2	1:E:225:ASP:N	2.27	0.44
1:C:12:VAL:HG11	1:C:114:ILE:HG23	1.97	0.44
1:C:52:GLN:CD	2:D:40:GLN:HE22	2.26	0.44
1:A:177:ASP:O	1:A:178:GLU:C	2.61	0.44
1:A:40:TYR:CZ	2:D:74:ARG:CG	3.00	0.44
1:C:25:TYR:CZ	1:C:64:ARG:HB3	2.53	0.44
1:C:246:TYR:OH	2:D:6:LYS:HE2	2.16	0.44
1:C:63:HIS:C	1:C:64:ARG:HG2	2.43	0.44
2:D:6:LYS:CG	2:D:12:THR:HG23	2.47	0.44
2:F:72:ARG:O	2:F:72:ARG:NH2	2.48	0.44
1:A:76:LEU:CD2	1:A:116:GLN:HB2	2.48	0.43
1:A:194:MET:CE	1:A:233:ALA:HB3	2.44	0.43
1:C:249:SER:HB2	1:C:266:LEU:HD21	1.99	0.43
1:E:76:LEU:HD21	1:E:116:GLN:HB2	2.00	0.43
1:A:177:ASP:C	1:A:179:THR:N	2.75	0.43
1:A:184:LEU:O	1:A:188:SER:OG	2.31	0.43
1:E:247:ILE:HB	1:E:274:VAL:HG13	2.01	0.43
2:B:62:GLN:O	2:B:65:SER:OG	2.29	0.43
1:A:26:THR:OG1	1:A:124:GLU:OE1	2.29	0.43
1:E:64:ARG:NH2	1:E:123:ARG:O	2.52	0.43
1:E:249:SER:HB2	1:E:266:LEU:HD21	2.00	0.43
1:C:76:LEU:N	1:C:76:LEU:HD23	2.33	0.43
1:E:282:LYS:O	1:E:286:GLN:HG3	2.18	0.43
1:C:27:GLU:HG3	1:C:124:GLU:CB	2.47	0.43
1:C:27:GLU:C	1:C:28:VAL:CG1	2.92	0.42
1:C:101:ILE:O	1:C:104:LEU:HB2	2.18	0.42
1:E:42:THR:HG23	1:E:44:ALA:O	2.19	0.42
2:B:6:LYS:CG	2:B:12:THR:HG23	2.49	0.42
1:A:258:GLU:N	1:A:258:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ILE:CD1	1:C:180:ALA:O	2.34	0.42
2:D:15:LEU:HD11	2:D:30:ILE:HG13	2.01	0.42
1:A:25:TYR:CE1	1:A:64:ARG:HB3	2.55	0.42
1:A:76:LEU:CD2	1:A:116:GLN:CB	2.98	0.42
1:E:94:ARG:HA	1:E:100:THR:HG22	2.02	0.42
1:A:192:ASP:O	1:A:195:ARG:NH1	2.46	0.41
1:C:107:GLN:HE21	1:C:111:LYS:NZ	2.17	0.41
1:C:112:LEU:CD1	1:C:181:GLU:HA	2.50	0.41
1:E:258:GLU:N	1:E:258:GLU:OE2	2.53	0.41
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.92	0.41
1:C:263:GLU:HA	1:C:266:LEU:HB2	2.01	0.41
1:A:40:TYR:CE2	2:D:74:ARG:HG2	2.55	0.41
1:C:27:GLU:OE2	1:C:135:ARG:NH1	2.37	0.41
1:C:112:LEU:HD12	1:C:181:GLU:HA	2.01	0.41
1:C:57:ILE:HG21	1:C:285:ALA:HB2	2.03	0.41
1:C:42:THR:HG23	1:C:44:ALA:O	2.21	0.41
2:D:1:MET:HE2	2:D:17:VAL:HG23	2.01	0.41
1:E:82:MET:HE1	1:E:187:LEU:HB3	2.03	0.41
1:A:52:GLN:HB3	1:A:66:ILE:HD12	2.02	0.41
1:A:171:ARG:HB3	1:A:174:ASP:CG	2.46	0.41
1:A:282:LYS:HA	1:A:282:LYS:HD2	1.88	0.41
1:C:107:GLN:HE22	1:C:111:LYS:CE	2.33	0.41
1:C:207:SER:HB2	1:C:210:VAL:HG22	2.01	0.41
1:A:280:ASP:OD2	1:A:282:LYS:HB3	2.21	0.41
2:B:43:LEU:HB3	2:B:50:LEU:HD12	2.02	0.41
1:C:76:LEU:HD21	1:C:116:GLN:HB2	2.02	0.41
1:A:83:TYR:CD2	1:A:109:LEU:HD22	2.55	0.41
1:C:86:ALA:HB3	1:C:101:ILE:HG22	2.03	0.41
1:A:63:HIS:C	1:A:64:ARG:HG2	2.46	0.40
1:A:42:THR:HG23	1:A:44:ALA:O	2.21	0.40
1:C:104:LEU:HD23	1:C:104:LEU:HA	1.93	0.40
1:C:127:ALA:HB1	1:C:129:TYR:CE1	2.57	0.40
1:C:219:GLN:HE21	1:C:268:ILE:HD13	1.86	0.40
1:E:192:ASP:O	1:E:195:ARG:NH1	2.47	0.40
1:A:66:ILE:O	1:A:66:ILE:HG22	2.21	0.40
1:C:87:LYS:HG2	1:C:102:ALA:HA	2.04	0.40
1:A:52:GLN:HG3	1:A:66:ILE:HD11	2.03	0.40
1:A:52:GLN:NE2	2:B:72:ARG:CB	2.85	0.40
1:A:76:LEU:HD13	1:A:113:ASN:HB3	2.04	0.40
1:A:282:LYS:O	1:A:286:GLN:HG3	2.21	0.40
1:C:147:TYR:CE1	1:C:152:LEU:HD11	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:PHE:O	1:C:225:ASP:HB2	2.22	0.40
1:A:82:MET:HE3	1:A:184:LEU:HD12	2.04	0.40
1:A:194:MET:CE	1:A:233:ALA:CB	2.99	0.40
1:C:15:TYR:CD1	1:C:15:TYR:C	2.99	0.40
1:C:282:LYS:HD2	1:C:282:LYS:HA	1.91	0.40

All (17) 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:103:ASP:N	1:C:103:ASP:CG[2_455]	0.66	1.54
1:C:103:ASP:CA	1:C:103:ASP:CG[2_455]	0.94	1.26
1:C:103:ASP:N	1:C:103:ASP:OD1[2_455]	1.25	0.95
1:C:102:ALA:C	1:C:103:ASP:OD1[2_455]	1.32	0.88
1:C:103:ASP:CA	1:C:103:ASP:OD2[2_455]	1.32	0.88
1:C:97:ASP:O	1:C:105:SER:OG[2_455]	1.44	0.76
1:C:103:ASP:CA	1:C:103:ASP:CB[2_455]	1.48	0.72
1:C:87:LYS:O	1:C:90:PRO:O[2_455]	1.53	0.67
1:C:103:ASP:N	1:C:103:ASP:CB[2_455]	1.61	0.59
1:C:103:ASP:N	1:C:103:ASP:OD2[2_455]	1.64	0.56
1:C:102:ALA:C	1:C:103:ASP:CG[2_455]	1.65	0.55
1:C:103:ASP:CB	1:C:103:ASP:CB[2_455]	1.75	0.45
1:C:94:ARG:NH1	1:C:104:LEU:O[2_455]	1.84	0.36
1:C:103:ASP:C	1:C:103:ASP:CG[2_455]	1.96	0.24
1:C:103:ASP:C	1:C:103:ASP:CB[2_455]	1.98	0.22
1:C:103:ASP:CA	1:C:103:ASP:OD1[2_455]	2.07	0.13
1:C:97:ASP:C	1:C:105:SER:OG[2_455]	2.09	0.11

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	306/343 (89%)	290 (95%)	14 (5%)	2 (1%)	18	18
1	C	306/343 (89%)	282 (92%)	23 (8%)	1 (0%)	36	41
1	E	306/343 (89%)	288 (94%)	18 (6%)	0	100	100
2	B	75/76 (99%)	72 (96%)	3 (4%)	0	100	100
2	D	75/76 (99%)	74 (99%)	1 (1%)	0	100	100
2	F	75/76 (99%)	73 (97%)	2 (3%)	0	100	100
All	All	1143/1257 (91%)	1079 (94%)	61 (5%)	3 (0%)	36	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	A	304	PRO
1	C	304	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	259/293 (88%)	245 (95%)	14 (5%)	20	23
1	C	259/293 (88%)	242 (93%)	17 (7%)	15	17
1	E	259/293 (88%)	247 (95%)	12 (5%)	24	30
2	B	69/68 (102%)	66 (96%)	3 (4%)	26	33
2	D	69/68 (102%)	66 (96%)	3 (4%)	26	33
2	F	69/68 (102%)	67 (97%)	2 (3%)	37	49
All	All	984/1083 (91%)	933 (95%)	51 (5%)	21	25

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	36	HIS

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Mol	Chain	Res	Type
1	A	52	GLN
1	A	58	ASP
1	A	76	LEU
1	A	135	ARG
1	A	188	SER
1	A	190	MET
1	A	193	LEU
1	A	215	PRO
1	A	236	LEU
1	A	260	ASP
1	A	274	VAL
1	A	282	LYS
2	B	1	MET
2	B	22	THR
2	B	64	GLU
1	C	52	GLN
1	C	59	ASP
1	C	76	LEU
1	C	101	ILE
1	C	103	ASP
1	C	104	LEU
1	C	107	GLN
1	C	126	GLU
1	C	159	LYS
1	C	172	ILE
1	C	193	LEU
1	C	215	PRO
1	C	216	THR
1	C	236	LEU
1	C	260	ASP
1	C	274	VAL
1	C	282	LYS
2	D	1	MET
2	D	38	PRO
2	D	39	ASP
1	E	3	SER
1	E	52	GLN
1	E	64	ARG
1	E	76	LEU
1	E	157	SER
1	E	193	LEU
1	E	208	ARG

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Mol	Chain	Res	Type
1	E	215	PRO
1	E	224	GLU
1	E	236	LEU
1	E	260	ASP
1	E	274	VAL
2	F	1	MET
2	F	64	GLU

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	63	HIS
1	A	80	GLN
1	A	91	HIS
1	A	113	ASN
1	A	116	GLN
1	A	309	GLN
2	B	40	GLN
2	B	41	GLN
1	C	36	HIS
1	C	91	HIS
1	C	107	GLN
2	D	40	GLN
2	D	60	ASN
2	D	62	GLN
1	E	36	HIS

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	308/343 (89%)	1.55	89 (28%) 1 1	28, 47, 83, 121	0
1	C	308/343 (89%)	1.57	96 (31%) 1 1	24, 48, 80, 105	0
1	E	308/343 (89%)	1.52	85 (27%) 1 1	26, 48, 77, 116	0
2	B	76/76 (100%)	1.70	25 (32%) 1 0	26, 52, 84, 109	1 (1%)
2	D	76/76 (100%)	0.98	10 (13%) 7 5	24, 46, 66, 74	1 (1%)
2	F	76/76 (100%)	1.58	27 (35%) 1 0	23, 54, 80, 100	1 (1%)
All	All	1152/1257 (91%)	1.52	332 (28%) 1 1	23, 48, 81, 121	3 (0%)

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	LEU	7.0
1	C	209	GLY	6.6
1	C	270	GLY	6.5
1	A	209	GLY	5.9
1	C	156	PHE	5.8
1	E	260	ASP	5.8
1	C	155	LEU	5.7
1	C	108	ASP	5.4
1	A	40	TYR	5.4
1	A	263	GLU	5.3
1	C	85	ALA	5.3
1	C	106	VAL	5.1
1	E	54	PHE	5.0
1	E	263	GLU	4.9
1	A	176	PHE	4.9
1	C	257	ILE	4.9
1	E	40	TYR	4.9
1	C	269	VAL	4.8
1	A	257	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	14	THR	4.8
1	A	256	GLY	4.8
1	C	254	HIS	4.7
1	C	117	LEU	4.7
1	C	179	THR	4.6
1	C	204	ILE	4.6
1	C	208	ARG	4.6
1	E	3	SER	4.6
1	E	35	ASN	4.6
1	E	34	TYR	4.5
1	E	51	LEU	4.5
2	B	20	SER	4.5
1	C	255	LEU	4.5
1	E	253	PRO	4.5
1	A	276	GLY	4.4
1	E	148	ALA	4.4
1	E	119	PHE	4.4
1	A	163	LEU	4.3
1	E	4	ILE	4.3
1	C	221	PHE	4.3
2	F	4	PHE	4.3
1	E	299	VAL	4.3
1	E	39	PRO	4.3
1	E	252	TRP	4.2
2	B	13	ILE	4.2
1	C	176	PHE	4.2
1	C	266	LEU	4.2
1	C	267	LYS	4.2
1	C	249	SER	4.1
1	E	294	CYS	4.1
1	E	47	THR	4.1
1	A	34	TYR	4.0
2	B	68	HIS	4.0
1	A	7	PRO	4.0
1	E	49	HIS	4.0
1	C	305	ASP	4.0
1	A	172	ILE	4.0
1	A	279	ALA	3.9
1	C	310	VAL	3.9
2	B	19	PRO	3.8
2	B	10	GLY	3.8
1	A	243	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	153	THR	3.8
1	A	156	PHE	3.8
1	A	39	PRO	3.7
1	E	271	SER	3.7
1	E	272	LEU	3.7
2	B	59	TYR	3.7
1	A	259	SER	3.7
1	E	261	ARG	3.7
1	E	248	SER	3.7
2	B	17	VAL	3.6
1	C	127	ALA	3.6
1	C	301	ILE	3.6
1	C	248	SER	3.6
1	E	156	PHE	3.6
1	C	259	SER	3.5
1	E	18	GLN	3.5
1	C	211	SER	3.5
2	F	56	LEU	3.5
1	E	129	TYR	3.5
1	E	172	ILE	3.5
1	C	213	ILE	3.5
1	E	10	LEU	3.5
1	E	175	ARG	3.4
1	A	183	TYR	3.4
1	C	172	ILE	3.4
1	A	37	LYS	3.4
1	C	146	ALA	3.4
1	C	154	HIS	3.4
1	E	199	PRO	3.4
2	F	59	TYR	3.4
1	A	255	LEU	3.3
2	F	1	MET	3.3
2	B	61	ILE	3.3
1	C	223	ARG	3.3
2	F	64	GLU	3.3
1	E	41	ALA	3.3
1	E	274	VAL	3.3
1	A	151	HIS	3.3
1	A	217	LEU	3.2
1	C	187	LEU	3.2
1	C	143	GLN	3.2
1	E	176	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	106	VAL	3.2
1	C	256	GLY	3.2
1	C	258	GLU	3.2
1	C	200	VAL	3.2
1	E	37	LYS	3.2
1	A	48	GLY	3.1
2	B	76	GLY	3.1
1	A	274	VAL	3.1
1	A	258	GLU	3.1
1	C	12	VAL	3.1
2	B	15	LEU	3.1
1	A	221	PHE	3.1
2	F	63	LYS	3.1
2	F	13	ILE	3.1
1	E	198	SER	3.1
1	A	162	VAL	3.1
1	A	154	HIS	3.0
2	F	8	LEU	3.0
1	C	247	ILE	3.0
1	E	213	ILE	3.0
1	A	277	GLN	3.0
1	C	125	SER	3.0
2	D	11[A]	LYS	3.0
1	C	260	ASP	3.0
1	E	96	ALA	3.0
1	E	141	ALA	3.0
1	A	41	ALA	2.9
1	C	291	VAL	2.9
1	A	3	SER	2.9
1	C	201	GLU	2.9
1	A	85	ALA	2.9
1	A	112	LEU	2.9
1	A	264	ARG	2.9
1	E	46	GLY	2.9
1	E	177	ASP	2.9
1	C	264	ARG	2.9
1	A	17	TYR	2.9
1	C	107	GLN	2.9
2	B	71	LEU	2.9
1	A	244	VAL	2.9
1	E	32	TRP	2.9
1	C	4	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	7	THR	2.9
2	F	61	ILE	2.9
1	C	52	GLN	2.8
1	C	112	LEU	2.8
1	E	291	VAL	2.8
2	D	13	ILE	2.8
1	E	115	ALA	2.8
1	A	106	VAL	2.8
1	A	210	VAL	2.8
2	B	26	VAL	2.8
1	E	206	HIS	2.8
1	E	259	SER	2.8
1	A	223	ARG	2.8
1	E	254	HIS	2.8
1	E	268	ILE	2.8
1	A	177	ASP	2.8
1	A	205	GLY	2.8
1	C	26	THR	2.7
1	E	143	GLN	2.7
1	A	130	GLY	2.7
1	A	212	GLY	2.7
1	E	98	GLY	2.7
2	D	65	SER	2.7
1	A	266	LEU	2.7
1	C	163	LEU	2.7
1	A	86	ALA	2.7
1	C	297	ALA	2.7
1	E	36	HIS	2.7
2	B	70	VAL	2.7
1	A	260	ASP	2.7
1	A	129	TYR	2.7
2	D	17	VAL	2.7
2	B	66	THR	2.7
1	A	114	ILE	2.7
1	C	268	ILE	2.7
1	E	235	SER	2.7
1	A	208	ARG	2.7
1	C	99	ARG	2.7
2	B	67	LEU	2.7
2	D	2	GLN	2.7
1	A	38	THR	2.7
1	C	251	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	153	THR	2.6
1	A	185	ILE	2.6
1	A	157	SER	2.6
1	C	250	SER	2.6
1	A	305	ASP	2.6
1	C	77	PHE	2.6
1	C	175	ARG	2.6
2	B	54	ARG	2.6
1	A	47	THR	2.6
1	A	218	ILE	2.6
1	E	86	ALA	2.6
1	C	203	PHE	2.6
1	E	38	THR	2.6
2	F	54	ARG	2.6
1	E	48	GLY	2.6
1	C	261	ARG	2.5
1	C	13	ALA	2.5
1	C	44	ALA	2.5
1	E	140	GLY	2.5
2	F	3	ILE	2.5
2	F	2	GLN	2.5
1	C	181	GLU	2.5
1	E	146	ALA	2.5
2	F	28	ALA	2.5
1	A	46	GLY	2.5
1	C	151	HIS	2.5
2	B	12	THR	2.5
1	A	271	SER	2.5
1	E	17	TYR	2.5
1	E	255	LEU	2.5
2	F	69	LEU	2.5
2	B	28	ALA	2.5
1	E	205	GLY	2.5
2	D	55	THR	2.5
1	E	128	SER	2.5
1	C	53	ARG	2.5
1	C	233	ALA	2.5
2	B	38	PRO	2.5
1	E	250	SER	2.4
1	E	204	ILE	2.4
2	F	23	ILE	2.4
1	C	5	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	109	LEU	2.4
1	E	154	HIS	2.4
1	A	281	ALA	2.4
1	C	141	ALA	2.4
1	A	98	GLY	2.4
1	C	253	PRO	2.4
1	A	100	THR	2.4
1	C	118	PHE	2.4
1	E	66	ILE	2.4
1	E	200	VAL	2.4
1	E	267	LYS	2.4
1	C	104	LEU	2.4
1	C	276	GLY	2.4
2	D	9	THR	2.4
1	C	152	LEU	2.4
1	A	149	ARG	2.4
1	A	246	TYR	2.4
1	E	94	ARG	2.4
1	C	177	ASP	2.4
2	F	55	THR	2.4
1	A	235	SER	2.4
2	B	1	MET	2.4
1	C	217	LEU	2.4
1	A	18	GLN	2.4
2	B	60	ASN	2.3
1	C	100	THR	2.3
2	F	66	THR	2.3
1	C	271	SER	2.3
1	A	262	VAL	2.3
1	A	254	HIS	2.3
1	E	107	GLN	2.3
1	E	93	HIS	2.3
2	F	30	ILE	2.3
1	C	76	LEU	2.3
1	C	113	ASN	2.3
1	C	252	TRP	2.3
2	F	22	THR	2.3
1	E	99	ARG	2.3
1	A	36	HIS	2.3
2	F	36	ILE	2.3
1	A	267	LYS	2.3
1	A	272	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	155	LEU	2.3
1	C	86	ALA	2.3
2	F	29	LYS	2.3
1	A	152	LEU	2.2
1	C	81	LEU	2.2
1	C	109	LEU	2.2
2	D	5	VAL	2.3
1	A	146	ALA	2.2
1	C	15	TYR	2.2
1	E	238	ALA	2.2
1	A	252	TRP	2.2
1	E	157	SER	2.2
1	E	12	VAL	2.2
2	F	19	PRO	2.2
2	B	75	GLY	2.2
1	A	42	THR	2.2
1	C	147	TYR	2.2
1	A	203	PHE	2.2
2	F	58	ASP	2.2
1	A	111	LYS	2.2
1	C	309	GLN	2.2
1	A	99	ARG	2.2
1	A	220	LEU	2.2
1	C	193	LEU	2.2
1	E	264	ARG	2.2
1	A	131	ASP	2.2
2	B	39	ASP	2.2
2	D	19	PRO	2.2
1	C	116	GLN	2.2
1	A	167	CYS	2.2
1	A	35	ASN	2.1
1	C	210	VAL	2.1
1	C	54	PHE	2.1
1	E	246	TYR	2.1
1	A	247	ILE	2.1
1	A	301	ILE	2.1
1	C	229	ILE	2.1
1	E	158	GLU	2.1
1	C	42	THR	2.1
1	E	53	ARG	2.1
1	A	233	ALA	2.1
1	A	273	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	136	TYR	2.1
1	C	93	HIS	2.1
1	C	73	MET	2.1
2	B	32	ASP	2.1
1	E	215	PRO	2.1
2	D	12	THR	2.0
1	C	8	GLU	2.0
1	A	280	ASP	2.0
1	C	164	TYR	2.0
2	F	70	VAL	2.0
1	E	212	GLY	2.0
2	F	47	GLY	2.0
1	E	237	PHE	2.0
1	A	153	THR	2.0
1	E	42	THR	2.0
1	A	102	ALA	2.0
1	A	52	GLN	2.0
1	E	138	LEU	2.0
2	F	67	LEU	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.