



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:37 PM UTC

PDB ID : 1URC / pdb_00001urc
Title : Cyclin A binding groove inhibitor Ace-Arg-Lys-Leu-Phe-Gly
Authors : Kontopidis, G.; Andrews, M.; McInnes, C.; Cowan, A.; Powers, H.; Innes, L.; Plater, A.; Griffiths, G.; Paterson, D.; Zheleva, D.; Lane, D.; Green, S.; Walkinshaw, M.; Fischer, P.
Deposited on : 2003-10-28
Resolution : 2.60 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
Mogul : 2022.3.0, CSD as543be (2022)
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

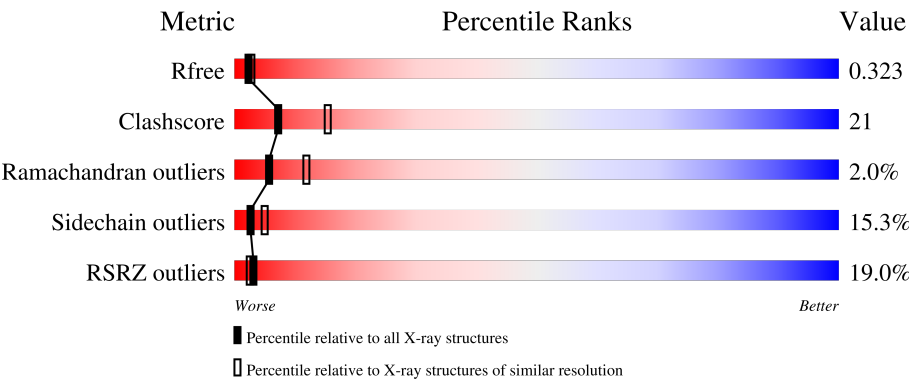
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	298	6% 60%30%5%5%
1	C	298	43% 57%31%8%
2	B	260	16% 59%32%7%
2	D	260	10% 63%29%7%
3	E	6	83%17%

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Mol	Chain	Length	Quality of chain
3	F	6	 50% 33% 17%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9357 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2378	1547	403	420	8			
1	C	297	Total	C	N	O	S	0	0	1
			2379	1547	404	420	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	1	0
			2087	1352	339	384	12			

- Molecule 3 is a protein called PEPTIDE INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			46	31	9	6			
3	F	6	Total	C	N	O	0	0	0
			46	31	9	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	75	Total	O	0	0
			75	75		
4	C	82	Total	O	0	0
			82	82		
4	D	95	Total	O	0	0
			95	95		

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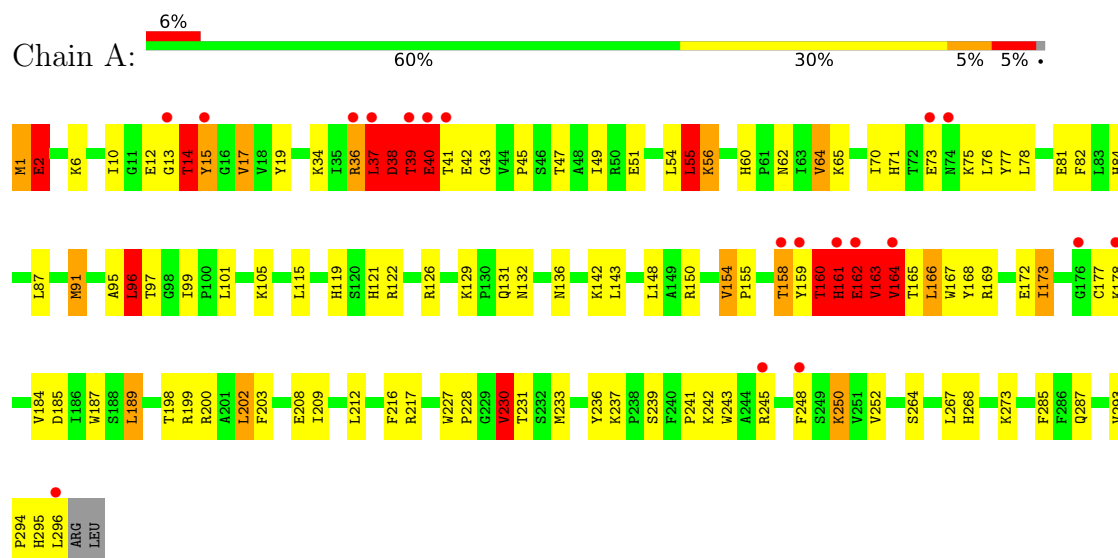
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	O	0	0
			1	1		
4	F	4	Total	O	0	0
			4	4		

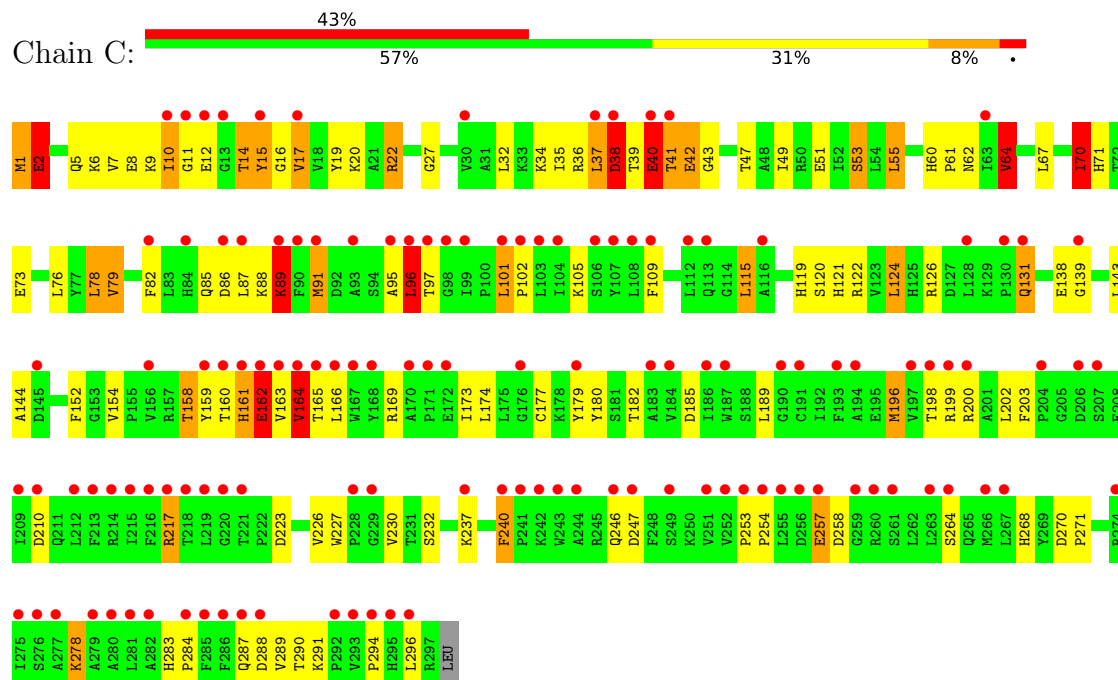
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

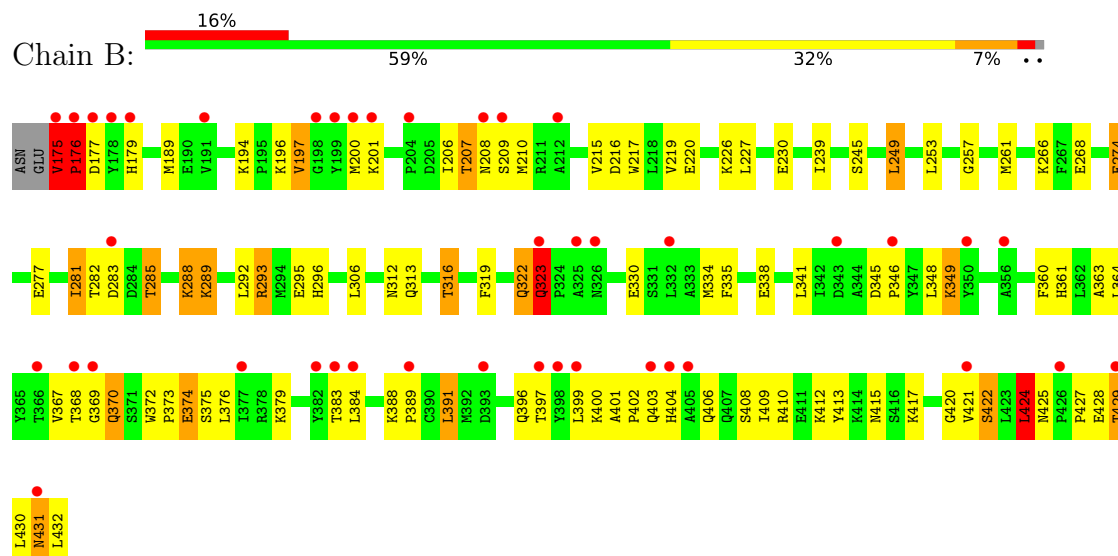
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



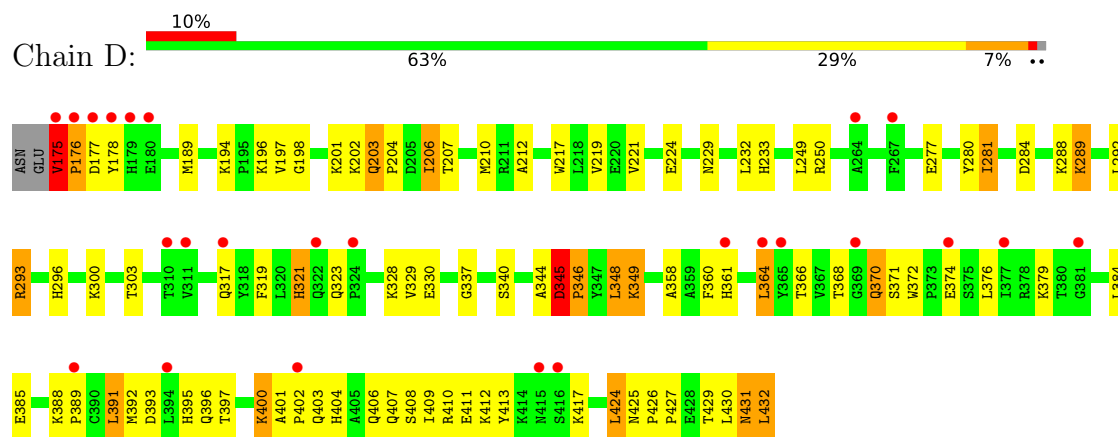
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



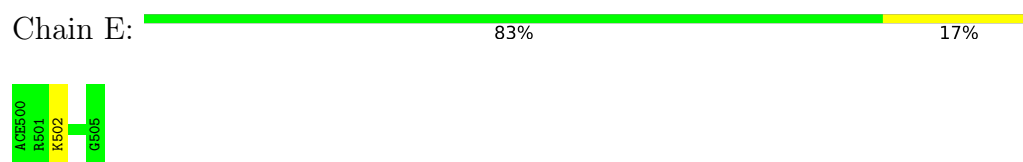
- Molecule 2: CYCLIN A2



- Molecule 2: CYCLIN A2



- Molecule 3: PEPTIDE INHIBITOR



- Molecule 3: PEPTIDE INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.63Å 113.51Å 155.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.00 – 2.60 14.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (14.00-2.60) 98.1 (14.00-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.56Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.254 0.288 , 0.323	Depositor DCC
R_{free} test set	1276 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	9357	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ACE

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	0.85	4/2440 (0.2%)	1.36	14/3313 (0.4%)
1	C	0.85	1/2441 (0.0%)	1.36	20/3315 (0.6%)
2	B	0.80	1/2133 (0.0%)	1.31	12/2896 (0.4%)
2	D	0.84	0/2142	1.34	9/2907 (0.3%)
3	E	0.83	0/44	2.17	0/56
3	F	0.72	0/44	2.15	3/56 (5.4%)
All	All	0.84	6/9244 (0.1%)	1.36	58/12543 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	C	0	6
2	B	0	1
2	D	0	2
All	All	0	16

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	200	MET	SD-CE	7.84	1.99	1.79
1	C	91	MET	SD-CE	-6.24	1.64	1.79
1	A	64	VAL	CA-CB	-6.07	1.48	1.54
1	A	39	THR	CA-CB	5.61	1.62	1.53
1	A	91	MET	SD-CE	-5.22	1.66	1.79
1	A	233	MET	SD-CE	5.15	1.92	1.79

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	THR	N-CA-C	-16.46	89.73	112.94
2	B	175	VAL	CA-C-N	9.41	131.60	119.84
2	B	175	VAL	C-N-CA	9.41	131.60	119.84
1	C	240	PHE	N-CA-C	-9.36	97.38	110.29
1	C	164	VAL	CB-CA-C	-8.02	98.13	111.29
1	A	39	THR	CB-CA-C	7.98	124.36	110.64
1	A	15	TYR	CB-CA-C	-7.80	96.31	109.65
2	B	219	VAL	N-CA-C	-7.48	103.17	110.72
1	A	82	PHE	N-CA-C	7.44	121.29	110.28
1	C	11	GLY	N-CA-C	7.05	120.71	110.63
1	A	14	THR	N-CA-C	-7.02	95.84	110.80
1	C	120	SER	N-CA-C	-6.95	104.77	113.18
1	C	109	PHE	N-CA-C	-6.92	103.82	111.36
2	B	176	PRO	N-CA-C	6.89	126.65	112.47
1	C	89	LYS	N-CA-C	-6.80	103.99	112.90
1	C	67	LEU	N-CA-C	6.66	118.62	111.36
2	D	175	VAL	CB-CA-C	-6.64	98.78	111.40
1	C	37	LEU	N-CA-C	6.59	120.95	112.12
2	B	215	VAL	N-CA-C	6.57	117.32	110.62
1	C	164	VAL	N-CA-C	6.49	122.85	109.34
1	C	42	GLU	N-CA-C	6.45	124.55	110.80
3	F	505	PHE	N-CA-CB	-6.39	102.51	112.41
1	A	230	VAL	CB-CA-C	-6.13	104.01	112.04
2	D	360	PHE	N-CA-C	-5.97	104.11	111.40
2	D	206	ILE	N-CA-C	5.94	118.54	108.86
1	C	257	GLU	N-CA-C	5.74	118.00	111.11
2	B	215	VAL	CB-CA-C	-5.73	104.40	112.14
1	C	64	VAL	CB-CA-C	-5.59	102.21	111.32
1	C	196	MET	N-CA-C	-5.57	105.36	111.82
2	B	399	LEU	N-CA-C	5.56	117.34	111.28
1	C	226	VAL	N-CA-C	5.55	116.28	110.62
1	A	55	LEU	N-CA-C	5.51	118.80	111.75
1	A	164	VAL	N-CA-C	5.46	120.70	109.34
1	C	10	ILE	N-CA-C	-5.46	107.81	113.10
2	D	203	GLN	CA-C-N	5.46	124.91	119.24
2	D	203	GLN	C-N-CA	5.46	124.91	119.24
1	A	54	LEU	N-CA-C	5.40	116.97	111.14
2	B	316	THR	OG1-CB-CG2	-5.38	98.54	109.30
1	A	162	GLU	N-CA-C	5.35	122.20	110.80
1	C	179	TYR	N-CA-C	5.33	117.93	109.50
2	B	253	LEU	N-CA-C	5.32	117.77	111.33
2	D	321	HIS	N-CA-C	-5.29	106.69	112.72
2	D	408	SER	N-CA-C	-5.27	106.11	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	502	ARG	N-CA-CB	-5.25	101.58	110.50
2	B	422	SER	N-CA-C	-5.24	106.89	113.28
1	C	79	VAL	N-CA-C	5.22	115.48	108.17
3	F	502	ARG	CG-CD-NE	-5.16	100.65	112.00
1	A	38	ASP	CA-C-O	5.12	125.95	120.32
1	C	14	THR	N-CA-C	5.12	118.62	112.38
1	A	267	LEU	N-CA-C	5.10	118.53	112.72
2	B	197	VAL	CB-CA-C	-5.09	103.87	112.16
1	C	258	ASP	O-C-N	-5.08	116.80	122.09
2	D	212	ALA	N-CA-C	5.07	117.19	111.11
2	D	393	ASP	N-CA-C	-5.07	105.83	111.36
1	C	16	GLY	N-CA-C	-5.05	106.07	112.54
2	B	397	THR	N-CA-C	-5.03	105.80	111.28
1	A	37	LEU	N-CA-C	-5.03	101.56	109.25
1	A	87	LEU	N-CA-C	-5.01	106.00	111.82

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
1	A	160	THR	Peptide
1	A	161	HIS	Peptide
1	A	162	GLU	Peptide
1	A	163	VAL	Peptide
1	A	38	ASP	Peptide
1	A	39	THR	Peptide
2	B	323	GLN	Peptide
1	C	161	HIS	Peptide
1	C	162	GLU	Peptide
1	C	164	VAL	Peptide
1	C	38	ASP	Peptide
1	C	40	GLU	Peptide
1	C	70	ILE	Peptide
2	D	194	LYS	Peptide
2	D	345	ASP	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	2378	0	2426	107	1
1	C	2379	0	2426	118	9
2	B	2083	0	2107	78	8
2	D	2087	0	2112	90	0
3	E	46	0	50	0	0
3	F	46	0	50	1	0
4	A	81	0	0	7	0
4	B	75	0	0	14	0
4	C	82	0	0	14	0
4	D	95	0	0	22	0
4	E	1	0	0	0	0
4	F	4	0	0	0	0
All	All	9357	0	9171	376	9

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 21.

All (376) 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)
2:B:175:VAL:HG22	2:B:176:PRO:CD	1.03	1.48
2:B:175:VAL:CG2	2:B:176:PRO:HD2	0.92	1.39
2:B:175:VAL:HG22	2:B:176:PRO:CG	1.55	1.34
2:B:175:VAL:CB	2:B:176:PRO:HD2	1.58	1.29
2:D:175:VAL:N	2:D:176:PRO:HD2	1.19	1.25
1:A:38:ASP:OD1	1:A:40:GLU:HG2	1.05	1.19
1:C:15:TYR:HB3	4:C:2009:HOH:O	1.36	1.19
2:D:175:VAL:N	2:D:176:PRO:CD	2.03	1.17
1:A:164:VAL:HG12	1:A:165:THR:N	1.49	1.15
1:C:164:VAL:HB	1:C:165:THR:HA	1.29	1.15
1:A:38:ASP:OD1	1:A:40:GLU:CG	1.96	1.13
1:A:164:VAL:CG1	1:A:165:THR:H	1.60	1.12
1:A:38:ASP:HA	1:A:39:THR:HG22	1.38	1.02
1:C:39:THR:O	1:C:40:GLU:CD	2.04	1.00
1:C:41:THR:HG22	2:D:288:LYS:HZ1	1.26	1.00
2:D:361:HIS:CE1	4:D:2069:HOH:O	2.14	1.00
1:C:51:GLU:O	1:C:55:LEU:HB2	1.63	0.98
2:B:175:VAL:CG2	2:B:176:PRO:CD	1.79	0.97
2:D:404:HIS:HD2	2:D:406:GLN:H	1.06	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ALA:O	1:A:96:LEU:HB3	1.67	0.95
2:B:175:VAL:HG23	2:B:176:PRO:HD2	1.47	0.94
1:C:268:HIS:HD2	4:C:2065:HOH:O	1.50	0.93
1:C:161:HIS:O	1:C:162:GLU:O	1.85	0.93
1:C:6:LYS:NZ	1:C:34:LYS:HZ2	1.67	0.92
1:A:209:ILE:HG22	4:A:2060:HOH:O	1.71	0.91
1:C:6:LYS:NZ	1:C:34:LYS:NZ	2.19	0.91
1:C:15:TYR:CD1	1:C:15:TYR:N	2.39	0.90
2:D:296:HIS:CD2	4:D:2054:HOH:O	2.25	0.90
1:C:41:THR:O	1:C:43:GLY:N	2.06	0.89
1:C:41:THR:HG22	2:D:288:LYS:NZ	1.88	0.88
1:C:15:TYR:CB	4:C:2009:HOH:O	1.99	0.87
1:C:40:GLU:O	1:C:40:GLU:HG2	1.71	0.87
2:B:175:VAL:HG22	2:B:176:PRO:HG2	1.54	0.86
1:C:15:TYR:CE1	1:C:47:THR:OG1	2.29	0.85
1:C:9:LYS:HD3	4:C:2004:HOH:O	1.77	0.85
1:C:164:VAL:CB	1:C:165:THR:HA	2.08	0.84
1:C:278:LYS:NZ	2:D:177:ASP:O	2.10	0.83
2:D:404:HIS:CD2	2:D:406:GLN:H	1.93	0.83
2:D:323:GLN:O	2:D:323:GLN:HG2	1.79	0.82
2:B:216:ASP:OD1	2:B:408:SER:HB2	1.79	0.81
1:A:245:ARG:HD3	4:A:2068:HOH:O	1.80	0.80
1:A:241:PRO:HG2	1:A:243:TRP:CZ3	2.16	0.80
1:C:95:ALA:O	1:C:96:LEU:HB3	1.80	0.80
1:A:38:ASP:HA	1:A:39:THR:CG2	2.13	0.79
1:C:164:VAL:HB	1:C:165:THR:CA	2.10	0.79
1:A:164:VAL:HG12	1:A:165:THR:H	1.14	0.78
1:A:1:MET:HE2	1:A:70:ILE:HD13	1.65	0.78
2:B:379:LYS:HE2	4:B:2052:HOH:O	1.83	0.78
1:C:6:LYS:HZ2	1:C:34:LYS:NZ	1.80	0.77
1:C:1:MET:CE	1:C:70:ILE:HD13	2.14	0.76
1:A:37:LEU:O	1:A:39:THR:HG22	1.85	0.76
1:A:250:LYS:HD2	4:A:2037:HOH:O	1.85	0.76
2:D:323:GLN:O	2:D:323:GLN:CG	2.32	0.76
2:B:430:LEU:HB3	2:B:432:LEU:CD2	2.15	0.76
1:A:1:MET:CE	1:A:70:ILE:HD13	2.15	0.76
1:A:252:VAL:O	1:A:252:VAL:HG23	1.83	0.76
2:B:277:GLU:O	2:B:281:ILE:HG23	1.86	0.75
1:A:13:GLY:C	1:A:14:THR:O	2.21	0.75
1:A:40:GLU:HG3	1:A:41:THR:N	2.01	0.75
1:C:41:THR:CG2	2:D:288:LYS:HZ1	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:THR:HG21	1:A:177:CYS:O	1.86	0.74
2:D:217:TRP:HZ2	2:D:281:ILE:HG13	1.50	0.74
2:B:249:LEU:HD22	1:C:27:GLY:HA3	1.67	0.74
1:A:115:LEU:HD22	1:A:119:HIS:CE1	2.23	0.74
1:A:13:GLY:O	1:A:14:THR:O	2.06	0.73
1:A:231:THR:HA	1:A:236:TYR:CD1	2.23	0.73
1:C:64:VAL:HG23	1:C:143:LEU:O	1.88	0.73
1:A:164:VAL:HG13	1:A:165:THR:H	1.52	0.73
1:C:91:MET:HE3	1:C:196:MET:HG2	1.68	0.73
1:C:37:LEU:C	1:C:39:THR:H	1.95	0.73
1:A:198:THR:O	1:A:199:ARG:HB2	1.88	0.72
1:C:1:MET:HE3	1:C:70:ILE:HD13	1.71	0.72
1:C:60:HIS:CD2	1:C:62:ASN:H	2.08	0.72
1:A:121:HIS:O	1:A:122:ARG:HG3	1.88	0.72
2:B:176:PRO:HD3	2:B:179:HIS:CE1	2.25	0.72
2:D:349:LYS:HE2	4:D:2068:HOH:O	1.88	0.72
2:B:288:LYS:HZ3	2:B:288:LYS:HB2	1.55	0.71
1:A:60:HIS:HD2	1:A:62:ASN:H	1.39	0.71
1:C:15:TYR:CE1	1:C:47:THR:CB	2.75	0.70
1:A:95:ALA:O	1:A:96:LEU:CB	2.39	0.69
2:D:346:PRO:O	2:D:349:LYS:HG3	1.92	0.69
2:B:217:TRP:HZ2	2:B:281:ILE:HG13	1.57	0.69
2:B:322:GLN:HG3	4:B:2043:HOH:O	1.92	0.69
1:C:39:THR:O	1:C:40:GLU:OE2	2.10	0.69
1:A:115:LEU:HD12	1:A:189:LEU:CD2	2.22	0.69
2:D:361:HIS:ND1	4:D:2069:HOH:O	2.18	0.68
2:D:207:THR:HG23	2:D:210[B]:MET:HE3	1.74	0.68
2:D:221:VAL:HG21	2:D:281:ILE:HD12	1.75	0.68
1:A:241:PRO:HG2	1:A:243:TRP:CH2	2.27	0.68
2:D:277:GLU:O	2:D:281:ILE:HG23	1.93	0.68
2:D:368:THR:OG1	2:D:370:GLN:HG3	1.94	0.68
2:B:266:LYS:NZ	2:B:295:GLU:OE2	2.27	0.67
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.77	0.67
2:B:274:GLU:HG2	4:B:2035:HOH:O	1.96	0.66
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.31	0.66
1:C:169:ARG:HD3	1:C:173:ILE:HG22	1.77	0.66
2:B:346:PRO:O	2:B:349:LYS:HG3	1.97	0.65
2:B:197:VAL:HG22	4:B:2018:HOH:O	1.97	0.65
2:B:363:ALA:O	2:B:367:VAL:HG23	1.95	0.65
1:A:15:TYR:CD2	1:A:47:THR:OG1	2.49	0.65
2:D:404:HIS:HD2	2:D:406:GLN:N	1.88	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LEU:C	1:C:39:THR:N	2.50	0.65
2:D:400:LYS:HE3	4:D:2083:HOH:O	1.96	0.65
1:A:227:TRP:O	1:A:230:VAL:HG22	1.97	0.64
1:C:39:THR:O	1:C:40:GLU:CG	2.44	0.64
1:C:7:VAL:HG12	1:C:8:GLU:HG2	1.81	0.63
1:A:159:TYR:O	1:A:160:THR:C	2.41	0.63
1:C:169:ARG:HD3	1:C:173:ILE:CG2	2.27	0.63
2:D:432:LEU:N	2:D:432:LEU:HD23	2.14	0.63
1:A:51:GLU:O	1:A:55:LEU:HB2	1.98	0.63
2:D:217:TRP:CZ2	2:D:281:ILE:HG13	2.34	0.62
1:A:73:GLU:HG3	1:C:2:GLU:HG2	1.82	0.62
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.35	0.62
1:C:41:THR:HA	2:D:288:LYS:HE3	1.80	0.62
1:C:95:ALA:O	1:C:96:LEU:CB	2.46	0.62
1:A:81:GLU:OE1	1:A:142:LYS:NZ	2.29	0.62
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.35	0.62
1:C:119:HIS:CE1	1:C:182:THR:HB	2.35	0.62
2:D:207:THR:HG23	2:D:210[B]:MET:CE	2.30	0.62
2:D:300:LYS:HB2	4:D:2055:HOH:O	1.99	0.61
2:B:207:THR:HG22	2:B:210:MET:HE3	1.83	0.61
1:C:20:LYS:HD2	1:C:82:PHE:CZ	2.36	0.61
2:D:175:VAL:O	2:D:175:VAL:HG13	1.94	0.61
1:A:231:THR:HG22	1:A:236:TYR:CE1	2.36	0.60
1:A:2:GLU:HG2	1:C:73:GLU:HG3	1.83	0.60
1:A:39:THR:H	1:A:40:GLU:HB3	1.67	0.60
2:D:210[A]:MET:HE1	2:D:250:ARG:CB	2.32	0.60
2:B:175:VAL:HG23	2:B:176:PRO:CD	2.14	0.60
1:A:60:HIS:CD2	1:A:62:ASN:H	2.18	0.60
2:D:210[A]:MET:CE	2:D:250:ARG:HB2	2.32	0.60
1:C:40:GLU:O	1:C:41:THR:O	2.19	0.60
1:C:41:THR:CG2	2:D:288:LYS:NZ	2.62	0.59
2:B:197:VAL:CG2	4:B:2018:HOH:O	2.51	0.59
1:A:121:HIS:C	1:A:122:ARG:HG3	2.27	0.59
2:B:293:ARG:HG3	2:B:293:ARG:HH11	1.67	0.59
1:C:32:LEU:HD22	1:C:79:VAL:HG22	1.85	0.59
1:C:105:LYS:NZ	1:C:288:ASP:OD1	2.34	0.59
1:C:253:PRO:N	1:C:254:PRO:CD	2.66	0.59
2:D:296:HIS:CG	4:D:2054:HOH:O	2.52	0.59
2:B:217:TRP:CZ2	2:B:281:ILE:HG13	2.37	0.58
1:C:6:LYS:NZ	1:C:34:LYS:HZ1	2.01	0.58
2:D:358:ALA:HA	2:D:391:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:TYR:HD2	1:A:47:THR:OG1	1.86	0.58
1:A:39:THR:H	1:A:40:GLU:CB	2.16	0.58
1:A:6:LYS:HZ1	1:A:34:LYS:HD2	1.69	0.58
2:D:379:LYS:HE2	4:D:2073:HOH:O	2.03	0.58
2:D:361:HIS:CG	4:D:2069:HOH:O	2.53	0.58
1:C:40:GLU:HB2	1:C:41:THR:OG1	2.03	0.58
2:B:430:LEU:HB3	2:B:432:LEU:HD23	1.86	0.58
1:C:53:SER:HB3	4:D:2058:HOH:O	2.03	0.58
1:C:41:THR:HG22	2:D:288:LYS:CE	2.35	0.57
2:B:175:VAL:CG2	2:B:176:PRO:HG2	2.29	0.57
1:C:51:GLU:HG3	1:C:55:LEU:HD22	1.87	0.57
2:D:319:PHE:CE2	2:D:330:GLU:HG2	2.40	0.57
1:A:164:VAL:HG12	1:A:165:THR:CA	2.33	0.56
1:A:17:VAL:CG1	1:A:19:TYR:CE2	2.88	0.56
2:B:293:ARG:HG3	2:B:293:ARG:NH1	2.20	0.56
1:C:159:TYR:HB3	1:C:162:GLU:HA	1.88	0.56
1:C:86:ASP:OD2	1:C:89:LYS:NZ	2.38	0.56
2:B:323:GLN:HE21	2:B:370:GLN:HE22	1.54	0.56
1:C:198:THR:O	1:C:199:ARG:HB2	2.06	0.55
1:A:81:GLU:CD	1:A:142:LYS:HZ3	2.13	0.55
1:C:64:VAL:CG2	1:C:143:LEU:O	2.55	0.55
2:D:395:HIS:HD2	4:D:2081:HOH:O	1.89	0.55
1:C:9:LYS:CD	4:C:2004:HOH:O	2.47	0.55
1:A:17:VAL:HG13	1:A:19:TYR:CE2	2.41	0.55
1:C:121:HIS:O	1:C:122:ARG:HG3	2.06	0.55
1:C:131:GLN:H	1:C:131:GLN:NE2	2.04	0.55
2:D:371:SER:O	2:D:372:TRP:C	2.50	0.54
2:B:207:THR:CG2	2:B:210:MET:HG3	2.37	0.54
2:D:303:THR:HG23	4:D:2057:HOH:O	2.06	0.54
1:A:2:GLU:HG3	4:C:2023:HOH:O	2.08	0.54
2:B:206:ILE:HA	2:B:210:MET:HE3	1.89	0.54
2:B:227:LEU:HD12	2:B:261:MET:HE3	1.90	0.54
2:D:337:GLY:O	2:D:340:SER:OG	2.23	0.54
1:C:60:HIS:HD2	1:C:62:ASN:H	1.52	0.54
1:A:159:TYR:HD2	1:A:163:VAL:HG13	1.73	0.54
1:C:78:LEU:HD23	1:C:78:LEU:N	2.22	0.54
1:C:162:GLU:OE1	1:C:180:TYR:OH	2.26	0.53
1:A:172:GLU:HG2	1:A:173:ILE:N	2.24	0.53
1:A:217:ARG:HD3	4:A:2062:HOH:O	2.07	0.53
1:C:6:LYS:HZ1	1:C:34:LYS:NZ	2.04	0.53
1:A:173:ILE:CD1	1:A:184:VAL:HG11	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:VAL:HG12	1:C:19:TYR:CE1	2.44	0.53
1:C:124:LEU:HD21	1:C:182:THR:HA	1.91	0.53
1:C:22:ARG:HD3	4:C:2010:HOH:O	2.07	0.52
1:C:164:VAL:CB	1:C:165:THR:CA	2.80	0.52
2:D:425:ASN:O	2:D:426:PRO:C	2.50	0.52
2:D:431:ASN:C	2:D:432:LEU:HD23	2.34	0.52
2:B:388:LYS:N	2:B:389:PRO:CD	2.73	0.52
1:A:81:GLU:CD	1:A:142:LYS:NZ	2.68	0.52
1:A:6:LYS:NZ	1:A:34:LYS:HD2	2.24	0.52
1:A:13:GLY:O	1:A:14:THR:C	2.52	0.52
1:C:37:LEU:O	1:C:38:ASP:C	2.53	0.52
1:A:1:MET:CE	1:A:70:ILE:CD1	2.87	0.52
1:A:71:HIS:CE1	2:B:296:HIS:CE1	2.98	0.52
1:C:161:HIS:C	1:C:162:GLU:O	2.48	0.52
2:D:345:ASP:OD2	2:D:346:PRO:HD2	2.10	0.52
2:B:312:ASN:OD1	2:B:334:MET:HE1	2.10	0.52
1:A:169:ARG:HD3	1:A:173:ILE:HG22	1.90	0.52
1:A:198:THR:O	1:A:199:ARG:CB	2.55	0.52
2:B:404:HIS:CD2	2:B:406:GLN:HB2	2.45	0.52
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.45	0.51
2:D:289:LYS:HG2	2:D:293:ARG:HD2	1.92	0.51
2:B:383:THR:O	2:B:384:LEU:C	2.54	0.51
2:D:289:LYS:HE3	4:D:2049:HOH:O	2.09	0.51
1:A:227:TRP:O	1:A:228:PRO:C	2.51	0.51
1:A:56:LYS:HD3	4:B:2040:HOH:O	2.10	0.51
1:C:71:HIS:CE1	2:D:296:HIS:NE2	2.79	0.51
1:A:56:LYS:CD	4:B:2040:HOH:O	2.59	0.50
1:C:9:LYS:CG	4:C:2004:HOH:O	2.58	0.50
1:A:294:PRO:HG2	1:A:296:LEU:HD13	1.93	0.50
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.47	0.50
1:C:290:THR:HG23	4:C:2073:HOH:O	2.12	0.50
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.94	0.50
2:D:233:HIS:HD2	4:D:2060:HOH:O	1.95	0.50
2:D:361:HIS:CD2	4:D:2069:HOH:O	2.65	0.50
2:D:379:LYS:CE	4:D:2073:HOH:O	2.60	0.50
1:A:166:LEU:O	1:A:167:TRP:HB2	2.12	0.49
2:D:430:LEU:O	2:D:431:ASN:CB	2.60	0.49
2:B:208:ASN:HB3	4:B:2022:HOH:O	2.12	0.49
2:D:361:HIS:CE1	2:D:384:LEU:HD11	2.48	0.49
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.94	0.49
2:B:319:PHE:CZ	2:B:330:GLU:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:THR:HG22	2:B:210:MET:CE	2.43	0.49
1:A:187:TRP:CD1	1:A:187:TRP:C	2.91	0.49
1:C:64:VAL:HG21	1:C:144:ALA:CB	2.42	0.49
1:C:253:PRO:N	1:C:254:PRO:HD3	2.28	0.49
1:C:71:HIS:CE1	2:D:296:HIS:CD2	3.01	0.48
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.94	0.48
1:C:10:ILE:HG21	1:C:20:LYS:HB2	1.95	0.48
1:A:73:GLU:CG	1:C:2:GLU:HG2	2.43	0.48
1:A:159:TYR:CD2	1:A:163:VAL:HG13	2.49	0.48
2:B:401:ALA:N	2:B:402:PRO:CD	2.77	0.48
1:C:32:LEU:CD2	1:C:79:VAL:HG22	2.42	0.48
1:A:166:LEU:O	1:A:168:TYR:N	2.42	0.48
2:D:210[A]:MET:HE1	2:D:250:ARG:HB3	1.96	0.48
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.49	0.48
1:A:56:LYS:HE2	4:B:2040:HOH:O	2.14	0.48
2:B:323:GLN:HE21	2:B:370:GLN:NE2	2.11	0.48
2:D:210[A]:MET:HE1	2:D:250:ARG:HB2	1.91	0.48
1:C:64:VAL:CG2	1:C:144:ALA:HB2	2.44	0.47
1:C:152:PHE:O	1:C:152:PHE:CD2	2.68	0.47
1:A:150:ARG:NH2	2:B:268:GLU:O	2.47	0.47
2:B:206:ILE:HA	2:B:210:MET:CE	2.44	0.47
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.44	0.47
2:B:282:THR:O	2:B:283:ASP:HB3	2.15	0.47
2:B:293:ARG:HH11	2:B:293:ARG:CG	2.27	0.47
2:D:210[B]:MET:HG2	3:F:505:PHE:CE2	2.49	0.47
2:D:329:VAL:HG11	2:D:364:LEU:HD13	1.95	0.47
2:D:345:ASP:OD2	2:D:346:PRO:CD	2.61	0.47
1:C:15:TYR:CE1	1:C:47:THR:HB	2.49	0.47
2:D:396:GLN:O	2:D:397:THR:C	2.58	0.47
1:A:49:ILE:CG2	2:B:306:LEU:HD12	2.44	0.47
1:C:15:TYR:HE1	1:C:47:THR:CB	2.26	0.47
1:C:101:LEU:N	1:C:102:PRO:CD	2.77	0.47
2:D:388:LYS:N	2:D:389:PRO:CD	2.78	0.47
1:A:115:LEU:HD12	1:A:189:LEU:HD22	1.96	0.47
1:A:43:GLY:HA2	4:A:2014:HOH:O	2.15	0.47
2:D:176:PRO:HB3	2:D:178:TYR:CZ	2.50	0.47
2:D:385:GLU:HB3	4:D:2076:HOH:O	2.14	0.47
2:B:415:ASN:ND2	4:B:2069:HOH:O	1.91	0.46
1:A:159:TYR:O	1:A:161:HIS:N	2.48	0.46
1:C:88:LYS:HD2	1:C:88:LYS:O	2.15	0.46
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:229:ASN:HB3	4:D:2067:HOH:O	2.14	0.46
1:A:173:ILE:CD1	1:A:184:VAL:CG1	2.94	0.46
1:A:77:TYR:C	1:A:78:LEU:HD23	2.41	0.46
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.98	0.46
2:B:175:VAL:CG2	2:B:176:PRO:CG	2.50	0.46
2:B:282:THR:O	2:B:285:THR:CG2	2.63	0.46
2:D:198:GLY:N	4:D:2015:HOH:O	2.48	0.46
2:D:395:HIS:HE1	2:D:427:PRO:O	1.98	0.46
2:B:430:LEU:O	2:B:432:LEU:HD22	2.16	0.46
1:C:6:LYS:HZ2	1:C:34:LYS:HZ1	1.56	0.46
2:D:303:THR:CG2	4:D:2057:HOH:O	2.64	0.46
1:C:91:MET:CE	1:C:196:MET:HG2	2.42	0.46
1:A:158:THR:HB	1:A:178:LYS:O	2.16	0.46
1:C:1:MET:CE	1:C:70:ILE:CD1	2.91	0.46
1:C:223:ASP:OD1	1:C:223:ASP:C	2.59	0.46
2:B:412:LYS:HE2	2:B:413:TYR:CE1	2.51	0.45
1:A:65:LYS:HD2	4:A:2030:HOH:O	2.16	0.45
1:A:136:ASN:C	1:A:136:ASN:OD1	2.59	0.45
1:A:129:LYS:HE2	1:A:132:ASN:ND2	2.31	0.45
2:D:366:THR:HG23	2:D:427:PRO:HD3	1.97	0.45
1:A:252:VAL:O	1:A:252:VAL:CG2	2.56	0.45
2:D:207:THR:N	2:D:210[B]:MET:HE3	2.31	0.45
2:B:175:VAL:CG2	2:B:176:PRO:HD3	2.19	0.45
2:B:421:VAL:O	2:B:424:LEU:HB2	2.17	0.45
1:A:173:ILE:HD13	1:A:184:VAL:CG1	2.47	0.45
2:D:321:HIS:CD2	2:D:376:LEU:HD21	2.52	0.45
2:B:207:THR:HG23	2:B:210:MET:HG3	1.99	0.45
2:D:410:ARG:O	2:D:411:GLU:C	2.59	0.45
1:A:78:LEU:HD23	1:A:78:LEU:N	2.31	0.44
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.77	0.44
1:C:115:LEU:HD11	1:C:185:ASP:HB3	1.98	0.44
2:B:335:PHE:CE1	2:B:409:ILE:HG22	2.51	0.44
2:B:410:ARG:NE	4:B:2067:HOH:O	2.51	0.44
1:C:158:THR:HG21	4:C:2048:HOH:O	2.17	0.44
2:D:412:LYS:HE2	2:D:413:TYR:CE1	2.52	0.44
2:D:204:PRO:HG2	4:D:2019:HOH:O	2.17	0.44
1:A:159:TYR:HB3	1:A:162:GLU:HA	1.99	0.44
1:A:169:ARG:HD3	1:A:173:ILE:CG2	2.47	0.44
1:C:202:LEU:HD23	1:C:203:PHE:CE2	2.51	0.44
1:C:95:ALA:O	1:C:96:LEU:HD23	2.18	0.44
2:D:403:GLN:O	2:D:404:HIS:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2044:HOH:O	2:D:317:GLN:HG2	2.17	0.44
1:C:15:TYR:CZ	1:C:47:THR:OG1	2.60	0.44
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.82	0.43
1:A:154:VAL:O	1:A:155:PRO:C	2.56	0.43
2:D:425:ASN:C	2:D:426:PRO:O	2.61	0.43
1:A:1:MET:N	1:A:2:GLU:OE2	2.31	0.43
2:B:373:PRO:HG2	2:B:376:LEU:HD12	2.00	0.43
1:C:121:HIS:C	1:C:122:ARG:HG3	2.43	0.43
1:A:212:LEU:HD22	1:A:216:PHE:CZ	2.54	0.43
2:B:335:PHE:HE1	2:B:409:ILE:HG22	1.84	0.43
2:D:207:THR:H	2:D:210[B]:MET:HE3	1.83	0.43
2:B:207:THR:OG1	2:B:208:ASN:N	2.52	0.43
1:C:159:TYR:CB	1:C:162:GLU:HA	2.49	0.43
2:B:404:HIS:HD2	2:B:406:GLN:H	1.67	0.43
2:D:361:HIS:CE1	2:D:384:LEU:CD1	3.02	0.43
2:B:427:PRO:HA	4:B:2073:HOH:O	2.19	0.43
2:D:175:VAL:O	2:D:176:PRO:O	2.36	0.42
1:A:64:VAL:HG12	1:A:143:LEU:O	2.19	0.42
1:A:105:LYS:HE2	1:A:285:PHE:CZ	2.54	0.42
1:C:40:GLU:C	1:C:41:THR:O	2.63	0.42
1:A:115:LEU:CD1	1:A:189:LEU:HD22	2.49	0.42
2:B:230:GLU:OE2	2:B:313:GLN:NE2	2.52	0.42
1:A:241:PRO:CG	1:A:243:TRP:CH2	3.00	0.42
2:D:203:GLN:HB3	2:D:206:ILE:HG12	2.00	0.42
2:D:401:ALA:HB3	2:D:402:PRO:HD3	2.01	0.42
1:A:115:LEU:HD12	1:A:189:LEU:HD23	1.98	0.42
1:C:14:THR:C	1:C:15:TYR:CD1	2.97	0.42
1:C:164:VAL:CG1	1:C:165:THR:HA	2.49	0.42
2:D:430:LEU:O	2:D:431:ASN:HB2	2.19	0.42
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.54	0.42
1:A:173:ILE:HD13	1:A:184:VAL:HG11	2.01	0.42
2:B:207:THR:HG22	2:B:210:MET:HG3	2.01	0.42
1:C:227:TRP:O	1:C:230:VAL:HG12	2.19	0.41
1:C:290:THR:CG2	4:C:2073:HOH:O	2.67	0.41
1:A:73:GLU:CD	1:C:2:GLU:HG2	2.45	0.41
2:B:282:THR:O	2:B:283:ASP:CB	2.67	0.41
2:B:396:GLN:HG3	4:B:2060:HOH:O	2.20	0.41
2:B:374:GLU:O	2:B:375:SER:C	2.64	0.41
2:B:429:THR:HA	4:B:2075:HOH:O	2.19	0.41
1:C:257:GLU:OE2	4:C:2062:HOH:O	2.21	0.41
2:B:289:LYS:HB2	2:B:289:LYS:HE2	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:GLN:NE2	1:C:89:LYS:HB3	2.35	0.41
1:C:270:ASP:OD1	1:C:271:PRO:HD2	2.19	0.41
2:B:239:ILE:HD11	2:B:257:GLY:HA2	2.02	0.41
2:B:372:TRP:HA	2:B:373:PRO:HD3	1.86	0.41
2:D:175:VAL:O	2:D:175:VAL:HG22	2.20	0.41
2:D:379:LYS:NZ	4:D:2073:HOH:O	2.47	0.41
1:A:212:LEU:HD22	1:A:216:PHE:CE1	2.55	0.41
2:B:430:LEU:O	2:B:431:ASN:HB2	2.20	0.41
1:C:174:LEU:O	4:C:2049:HOH:O	2.22	0.41
1:A:36:ARG:HH11	1:A:36:ARG:HD3	1.73	0.41
1:A:115:LEU:HD11	1:A:185:ASP:HB3	2.03	0.41
2:D:407:GLN:O	2:D:411:GLU:HG2	2.21	0.41
2:B:338:GLU:O	2:B:341:LEU:HB2	2.21	0.41
1:A:15:TYR:CE2	1:A:45:PRO:HB3	2.56	0.41
2:B:368:THR:OG1	2:B:370:GLN:HG3	2.21	0.41
1:C:105:LYS:HG2	1:C:289:VAL:HG23	2.03	0.41
2:D:219:VAL:HG21	2:D:409:ILE:CG1	2.51	0.41
1:A:173:ILE:HD11	1:A:184:VAL:HG11	2.03	0.41
1:C:164:VAL:H	1:C:164:VAL:HG22	1.41	0.41
1:A:239:SER:HB3	4:A:2067:HOH:O	2.21	0.40
1:C:15:TYR:CD2	1:C:35:ILE:HG12	2.56	0.40
2:D:388:LYS:N	2:D:389:PRO:HD2	2.37	0.40
2:B:361:HIS:HD2	2:B:391:LEU:HD21	1.83	0.40
1:C:49:ILE:HG23	1:C:49:ILE:HD12	1.72	0.40
2:B:360:PHE:O	2:B:364:LEU:HB2	2.21	0.40
1:C:17:VAL:CG1	1:C:19:TYR:CE1	3.05	0.40
2:D:206:ILE:HG21	2:D:206:ILE:HD13	1.71	0.40
1:C:60:HIS:HA	1:C:61:PRO:HD3	1.88	0.40
2:D:280:TYR:CD2	2:D:280:TYR:C	2.99	0.40

All (9) 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)
2:B:431:ASN:CG	1:C:210:ASP:OD1[2_664]	1.25	0.95
2:B:431:ASN:ND2	1:C:210:ASP:OD1[2_664]	1.46	0.74
2:B:428:GLU:OE2	1:C:237:LYS:NZ[2_664]	1.65	0.55
2:B:369:GLY:O	1:C:217:ARG:NE[2_664]	1.75	0.45
2:B:431:ASN:CB	1:C:210:ASP:OD1[2_664]	1.93	0.27
2:B:431:ASN:ND2	1:C:210:ASP:CA[2_664]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:ASN:ND2	1:C:210:ASP:CG[2_664]	2.06	0.14
2:B:431:ASN:OD1	1:C:210:ASP:OD1[2_664]	2.07	0.13
1:A:84:HIS:ND1	1:C:287:GLN:O[1_455]	2.15	0.05

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	294/298 (99%)	268 (91%)	19 (6%)	7 (2%)	4	9
1	C	295/298 (99%)	274 (93%)	12 (4%)	9 (3%)	3	5
2	B	256/260 (98%)	244 (95%)	9 (4%)	3 (1%)	10	23
2	D	257/260 (99%)	236 (92%)	18 (7%)	3 (1%)	10	23
3	E	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
3	F	4/6 (67%)	4 (100%)	0	0	100	100
All	All	1110/1128 (98%)	1029 (93%)	59 (5%)	22 (2%)	6	12

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	160	THR
1	A	162	GLU
2	B	176	PRO
2	B	424	LEU
1	C	38	ASP
1	C	41	THR
1	C	42	GLU
1	C	162	GLU
2	D	176	PRO
1	A	2	GLU
1	A	96	LEU

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Mol	Chain	Res	Type
1	A	164	VAL
2	B	420	GLY
1	C	2	GLU
1	C	96	LEU
1	C	164	VAL
2	D	424	LEU
1	C	160	THR
1	A	14	THR
1	C	40	GLU
2	D	346	PRO

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	261/263 (99%)	219 (84%)	42 (16%)	2	4
1	C	261/263 (99%)	218 (84%)	43 (16%)	2	4
2	B	232/234 (99%)	196 (84%)	36 (16%)	2	5
2	D	233/234 (100%)	204 (88%)	29 (12%)	4	9
3	E	4/4 (100%)	3 (75%)	1 (25%)	0	1
3	F	4/4 (100%)	3 (75%)	1 (25%)	0	1
All	All	995/1002 (99%)	843 (85%)	152 (15%)	3	5

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	10	ILE
1	A	12	GLU
1	A	14	THR
1	A	17	VAL
1	A	36	ARG
1	A	37	LEU
1	A	39	THR

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Mol	Chain	Res	Type
1	A	40	GLU
1	A	42	GLU
1	A	55	LEU
1	A	56	LYS
1	A	75	LYS
1	A	76	LEU
1	A	96	LEU
1	A	97	THR
1	A	101	LEU
1	A	126	ARG
1	A	131	GLN
1	A	148	LEU
1	A	154	VAL
1	A	158	THR
1	A	160	THR
1	A	161	HIS
1	A	163	VAL
1	A	166	LEU
1	A	173	ILE
1	A	189	LEU
1	A	200	ARG
1	A	202	LEU
1	A	208	GLU
1	A	230	VAL
1	A	237	LYS
1	A	242	LYS
1	A	248	PHE
1	A	250	LYS
1	A	264	SER
1	A	268	HIS
1	A	273	LYS
1	A	287	GLN
1	A	293	VAL
1	A	295	HIS
2	B	175	VAL
2	B	177	ASP
2	B	189	MET
2	B	194	LYS
2	B	196	LYS
2	B	201	LYS
2	B	207	THR
2	B	209	SER

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Mol	Chain	Res	Type
2	B	220	GLU
2	B	226	LYS
2	B	245	SER
2	B	249	LEU
2	B	274	GLU
2	B	281	ILE
2	B	285	THR
2	B	288	LYS
2	B	289	LYS
2	B	292	LEU
2	B	293	ARG
2	B	316	THR
2	B	322	GLN
2	B	323	GLN
2	B	345	ASP
2	B	348	LEU
2	B	349	LYS
2	B	370	GLN
2	B	374	GLU
2	B	391	LEU
2	B	400	LYS
2	B	403	GLN
2	B	417	LYS
2	B	422	SER
2	B	424	LEU
2	B	425	ASN
2	B	429	THR
2	B	431	ASN
1	C	1	MET
1	C	2	GLU
1	C	5	GLN
1	C	12	GLU
1	C	15	TYR
1	C	17	VAL
1	C	22	ARG
1	C	36	ARG
1	C	38	ASP
1	C	40	GLU
1	C	53	SER
1	C	55	LEU
1	C	64	VAL
1	C	70	ILE

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Mol	Chain	Res	Type
1	C	76	LEU
1	C	78	LEU
1	C	87	LEU
1	C	89	LYS
1	C	96	LEU
1	C	97	THR
1	C	101	LEU
1	C	115	LEU
1	C	124	LEU
1	C	126	ARG
1	C	131	GLN
1	C	138	GLU
1	C	154	VAL
1	C	158	THR
1	C	163	VAL
1	C	164	VAL
1	C	166	LEU
1	C	177	CYS
1	C	189	LEU
1	C	200	ARG
1	C	217	ARG
1	C	232	SER
1	C	240	PHE
1	C	246	GLN
1	C	247	ASP
1	C	264	SER
1	C	278	LYS
1	C	291	LYS
1	C	296	LEU
2	D	175	VAL
2	D	189	MET
2	D	196	LYS
2	D	197	VAL
2	D	201	LYS
2	D	202	LYS
2	D	224	GLU
2	D	232	LEU
2	D	249	LEU
2	D	281	ILE
2	D	284	ASP
2	D	289	LYS
2	D	292	LEU

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Mol	Chain	Res	Type
2	D	293	ARG
2	D	328	LYS
2	D	345	ASP
2	D	348	LEU
2	D	349	LYS
2	D	364	LEU
2	D	370	GLN
2	D	374	GLU
2	D	391	LEU
2	D	392	MET
2	D	400	LYS
2	D	417	LYS
2	D	424	LEU
2	D	429	THR
2	D	431	ASN
2	D	432	LEU
3	E	502	LYS
3	F	503	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
1	A	265	GLN
1	A	268	HIS
2	B	179	HIS
2	B	208	ASN
2	B	296	HIS
2	B	322	GLN
2	B	370	GLN
2	B	404	HIS
2	B	431	ASN
1	C	60	HIS
1	C	71	HIS
1	C	84	HIS
1	C	85	GLN
1	C	121	HIS
1	C	131	GLN
1	C	287	GLN
2	D	208	ASN
2	D	233	HIS

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Mol	Chain	Res	Type
2	D	322	GLN
2	D	326	ASN
2	D	370	GLN
2	D	395	HIS
2	D	404	HIS
2	D	419	HIS
2	D	431	ASN

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	296/298 (99%)	0.49	19 (6%) 25 20	23, 40, 83, 112	1 (0%)
1	C	297/298 (99%)	1.91	127 (42%) 0 0	21, 40, 84, 111	0
2	B	258/260 (99%)	1.19	42 (16%) 4 3	23, 42, 69, 101	0
2	D	258/260 (99%)	0.84	25 (9%) 13 10	25, 43, 70, 102	1 (0%)
3	E	5/6 (83%)	1.15	0 100 100	40, 41, 57, 76	0
3	F	5/6 (83%)	0.36	0 100 100	40, 43, 50, 58	0
All	All	1119/1128 (99%)	1.11	213 (19%) 3 2	21, 41, 79, 112	2 (0%)

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	ARG	5.1
1	C	194	ALA	5.1
2	B	175	VAL	4.6
1	C	218	THR	4.6
1	C	284	PRO	4.4
1	C	213	PHE	4.3
1	C	287	GLN	4.2
1	A	40	GLU	4.2
1	C	168	TYR	4.2
1	A	73	GLU	4.1
1	C	276	SER	4.0
1	C	220	GLY	4.0
1	C	243	TRP	3.9
1	C	254	PRO	3.9
2	D	179	HIS	3.8
1	C	187	TRP	3.7
2	B	200	MET	3.7
1	C	191	CYS	3.6
1	C	163	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	256	ASP	3.6
1	C	90	PHE	3.6
2	B	201	LYS	3.6
1	C	253	PRO	3.5
2	D	175	VAL	3.5
1	C	249	SER	3.5
1	C	183	ALA	3.5
1	C	277	ALA	3.5
1	C	107	TYR	3.5
1	C	210	ASP	3.5
1	C	86	ASP	3.5
2	D	364	LEU	3.4
1	C	159	TYR	3.3
2	B	346	PRO	3.3
1	C	216	PHE	3.3
1	C	162	GLU	3.3
1	C	206	ASP	3.3
1	A	41	THR	3.2
1	C	139	GLY	3.2
1	C	197	VAL	3.2
1	C	104	ILE	3.2
1	C	285	PHE	3.2
1	A	13	GLY	3.2
1	C	109	PHE	3.2
1	C	296	LEU	3.1
1	C	241	PRO	3.1
1	C	108	LEU	3.1
1	C	130	PRO	3.1
1	C	204	PRO	3.1
1	C	95	ALA	3.1
1	C	193	PHE	3.1
1	C	281	LEU	3.1
1	C	261	SER	3.1
1	C	15	TYR	3.0
1	C	255	LEU	3.0
1	C	244	ALA	3.0
1	C	294	PRO	3.0
2	B	212	ALA	3.0
1	C	106	SER	2.9
1	C	165	THR	2.9
2	B	325	ALA	2.9
2	D	178	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	128	LEU	2.9
2	B	404	HIS	2.9
1	C	252	VAL	2.8
1	C	37	LEU	2.8
2	B	397	THR	2.8
1	C	161	HIS	2.8
1	C	293	VAL	2.8
1	C	170	ALA	2.8
1	C	280	ALA	2.8
1	C	240	PHE	2.8
2	D	180	GLU	2.8
2	B	398	TYR	2.8
1	C	246	GLN	2.7
1	A	37	LEU	2.7
2	B	369	GLY	2.7
2	D	415	ASN	2.7
1	A	36	ARG	2.7
1	C	40	GLU	2.7
1	C	266	MET	2.7
1	C	199	ARG	2.7
2	B	431	ASN	2.7
1	C	282	ALA	2.7
1	C	279	ALA	2.6
1	C	288	ASP	2.6
2	B	283	ASP	2.6
2	D	322	GLN	2.6
1	C	63	ILE	2.6
2	D	374	GLU	2.6
2	D	381	GLY	2.6
1	C	164	VAL	2.6
1	C	286	PHE	2.6
1	C	113	GLN	2.6
2	B	389	PRO	2.6
1	C	242	LYS	2.6
1	C	184	VAL	2.6
1	C	87	LEU	2.5
1	C	219	LEU	2.5
2	D	317	GLN	2.5
1	C	96	LEU	2.5
1	C	41	THR	2.5
1	C	97	THR	2.5
1	C	221	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	38	ASP	2.5
1	C	263	LEU	2.5
2	B	176	PRO	2.5
2	B	383	THR	2.5
1	C	251	VAL	2.5
2	B	366	THR	2.4
1	A	296	LEU	2.4
1	C	167	TRP	2.4
1	C	13	GLY	2.4
2	D	324	PRO	2.4
2	D	369	GLY	2.4
1	C	101	LEU	2.4
1	C	176	GLY	2.4
1	C	93	ALA	2.4
1	C	116	ALA	2.4
1	C	160	THR	2.4
1	C	209	ILE	2.4
1	C	84	HIS	2.4
2	D	416	SER	2.4
1	C	12	GLU	2.4
1	C	145	ASP	2.4
1	C	259	GLY	2.4
1	C	292	PRO	2.4
1	C	247	ASP	2.4
1	A	15	TYR	2.3
1	C	166	LEU	2.3
1	C	267	LEU	2.3
1	A	74	ASN	2.3
1	A	176	GLY	2.3
1	C	131	GLN	2.3
1	C	200	ARG	2.3
1	A	159	TYR	2.3
2	D	310	THR	2.3
1	C	91	MET	2.3
2	B	209	SER	2.3
2	B	426	PRO	2.3
1	A	248	PHE	2.3
2	D	361	HIS	2.3
2	B	350	TYR	2.3
2	B	382	TYR	2.3
2	B	204	PRO	2.3
2	D	176	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	323	GLN	2.3
1	C	237	LYS	2.3
1	A	162	GLU	2.3
1	C	172	GLU	2.3
1	C	214	ARG	2.3
2	B	393	ASP	2.3
1	C	156	VAL	2.3
2	B	332	LEU	2.3
1	C	82	PHE	2.3
2	B	356	ALA	2.2
1	C	264	SER	2.2
2	D	177	ASP	2.2
2	D	394	LEU	2.2
1	C	89	LYS	2.2
1	C	207	SER	2.2
1	C	229	GLY	2.2
1	C	10	ILE	2.2
1	C	215	ILE	2.2
2	D	267	PHE	2.2
2	B	368	THR	2.2
2	D	365	TYR	2.2
1	C	171	PRO	2.2
1	C	295	HIS	2.2
1	C	198	THR	2.2
1	C	228	PRO	2.2
2	B	384	LEU	2.2
1	A	39	THR	2.1
1	C	260	ARG	2.1
1	C	11	GLY	2.1
1	C	98	GLY	2.1
2	B	421	VAL	2.1
2	B	405	ALA	2.1
2	D	264	ALA	2.1
1	A	245	ARG	2.1
2	B	326	ASN	2.1
2	B	403	GLN	2.1
1	C	103	LEU	2.1
1	C	179	TYR	2.1
2	B	198	GLY	2.1
1	C	17	VAL	2.1
2	B	191	VAL	2.1
1	C	274	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	112	LEU	2.1
2	B	208	ASN	2.1
2	B	179	HIS	2.1
2	B	199	TYR	2.1
1	C	186	ILE	2.1
1	C	275	ILE	2.1
2	B	177	ASP	2.1
1	C	102	PRO	2.1
2	D	402	PRO	2.1
1	C	212	LEU	2.1
1	C	190	GLY	2.1
1	A	164	VAL	2.1
2	D	311	VAL	2.1
1	C	257	GLU	2.0
1	A	178	LYS	2.0
1	A	158	THR	2.0
2	D	389	PRO	2.0
1	C	99	ILE	2.0
2	B	377	ILE	2.0
2	B	343	ASP	2.0
2	B	429	THR	2.0
2	B	399	LEU	2.0
1	A	161	HIS	2.0
2	D	377	ILE	2.0
1	C	30	VAL	2.0
2	B	178	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.