



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:41 PM UTC

PDB ID : 2D0I / pdb_00002d0i
Title : Crystal Structure PH0520 protein from *Pyrococcus horikoshii* OT3
Authors : Lokanath, N.K.; Terao, Y.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-08-02
Resolution : 1.95 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

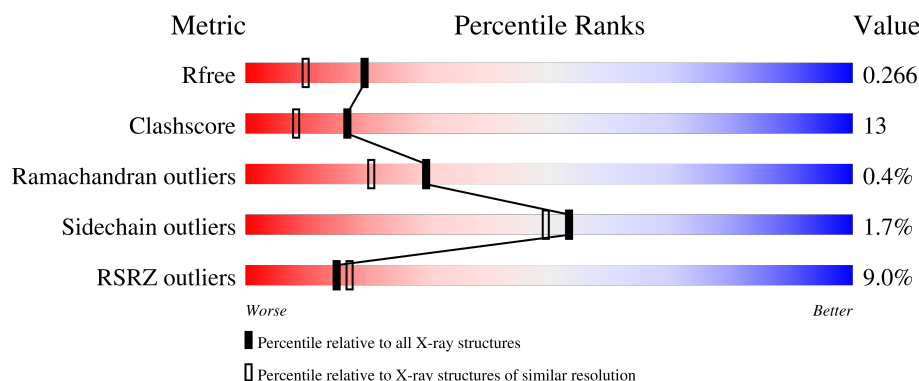
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	333	5% 75% 23% .
1	B	333	5% 83% 15% .
1	C	333	20% 65% 34% .
1	D	333	6% 73% 25% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11762 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 dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2683	1728	462	486	7			
1	B	333	Total	C	N	O	S	0	0	0
			2683	1728	462	486	7			
1	C	333	Total	C	N	O	S	0	0	0
			2683	1728	462	486	7			
1	D	333	Total	C	N	O	S	0	0	0
			2683	1728	462	486	7			

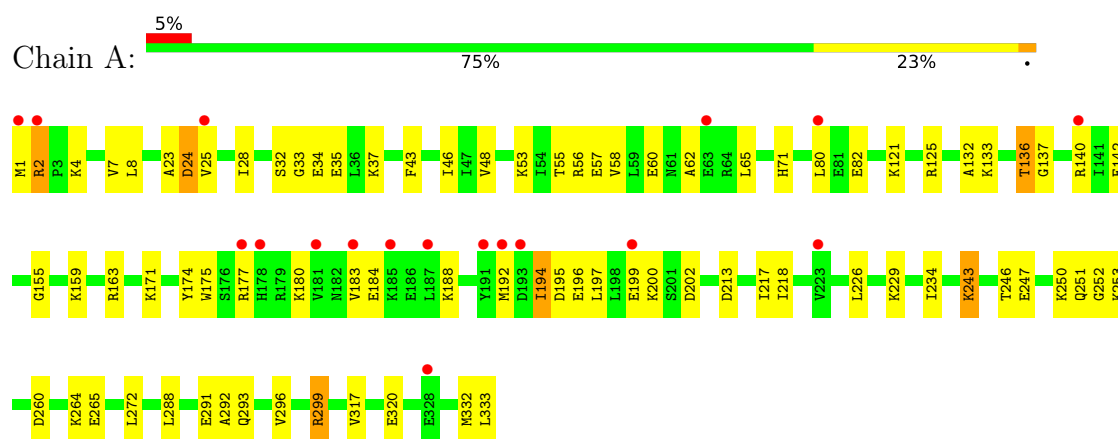
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	254	Total	O	0	0
			254	254		
2	B	299	Total	O	0	0
			299	299		
2	C	218	Total	O	0	0
			218	218		
2	D	259	Total	O	0	0
			259	259		

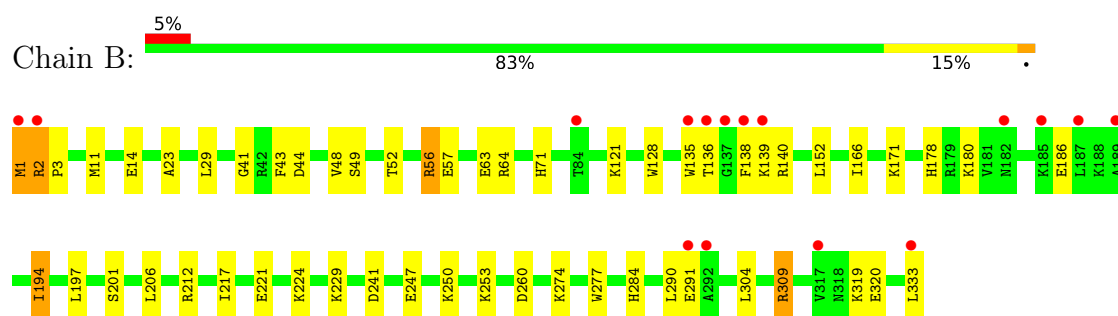
3 Residue-property plots

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.

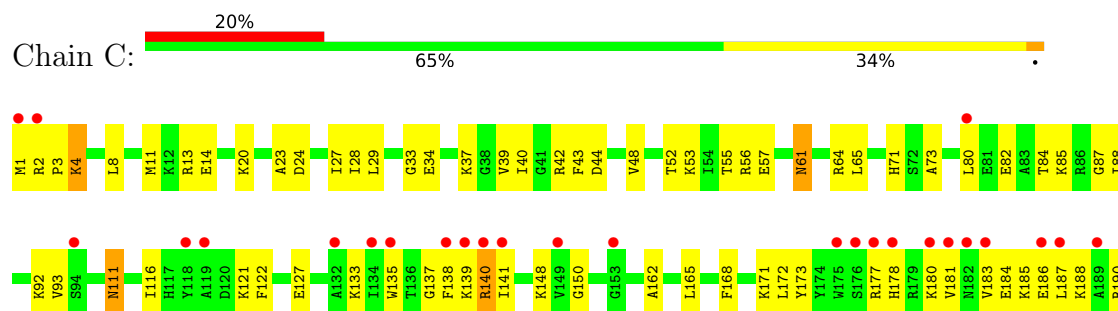
• Molecule 1: dehydrogenase

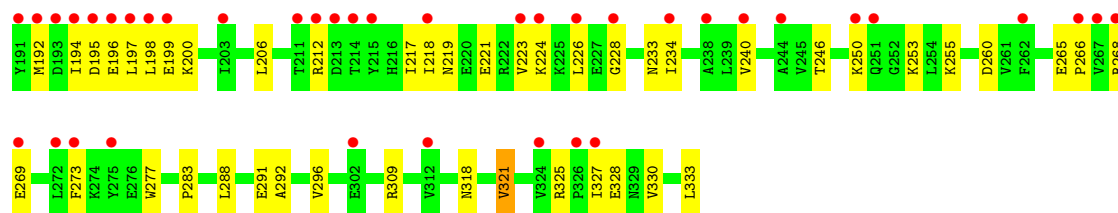


• Molecule 1: dehydrogenase

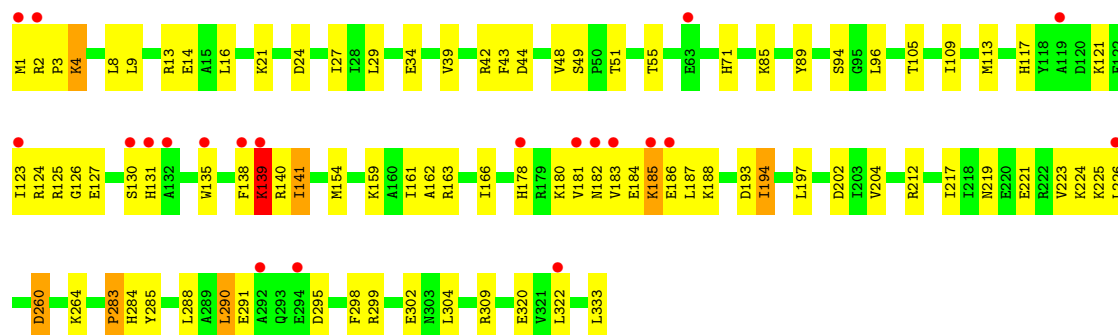
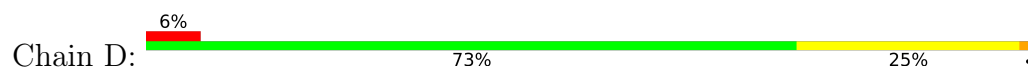


• Molecule 1: dehydrogenase





● Molecule 1: dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.76Å 63.74Å 131.98Å 90.00° 103.14° 90.00°	Depositor
Resolution (Å)	34.69 – 1.95 34.69 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.0 (34.69-1.95) 93.6 (34.69-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.92Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.265 0.234 , 0.266	Depositor DCC
R_{free} test set	5320 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11762	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 45.15 % 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 1.3782e-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	0.47	0/2728	0.96	8/3669 (0.2%)
1	B	0.41	0/2728	0.94	10/3669 (0.3%)
1	C	0.43	0/2728	0.96	11/3669 (0.3%)
1	D	0.44	0/2728	0.96	9/3669 (0.2%)
All	All	0.44	0/10912	0.96	38/14676 (0.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	HIS	N-CA-CB	-9.49	98.50	110.45
1	A	43	PHE	N-CA-C	7.66	121.92	109.59
1	B	43	PHE	N-CA-C	7.35	121.82	109.76
1	D	43	PHE	N-CA-C	7.02	121.28	109.76
1	D	29	LEU	N-CA-C	6.89	119.07	109.15
1	C	29	LEU	N-CA-C	6.77	119.54	109.59
1	C	43	PHE	N-CA-C	6.65	120.08	109.24
1	D	283	PRO	N-CA-CB	6.58	107.14	102.79
1	D	202	ASP	N-CA-C	-6.48	105.51	113.41
1	B	29	LEU	N-CA-C	6.13	119.10	109.96
1	C	260	ASP	N-CA-C	-6.04	105.87	113.72
1	D	139	LYS	N-CA-C	5.78	117.25	111.07
1	A	260	ASP	N-CA-C	-5.76	106.23	113.72
1	A	24	ASP	N-CA-C	-5.70	101.20	110.20
1	B	166	ILE	CB-CA-C	-5.56	108.42	113.70
1	A	2	ARG	CA-C-N	-5.55	114.24	119.85
1	A	2	ARG	C-N-CA	-5.55	114.24	119.85
1	D	44	ASP	N-CA-C	-5.54	106.36	113.23
1	C	44	ASP	N-CA-C	-5.53	106.04	112.89
1	A	202	ASP	N-CA-C	-5.41	105.82	112.90
1	C	172	LEU	N-CA-C	5.33	117.93	109.24
1	C	177	ARG	O-C-N	5.33	127.63	122.09
1	B	44	ASP	N-CA-C	-5.31	105.54	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	ARG	N-CA-C	-5.31	106.39	112.92
1	B	136	THR	N-CA-C	-5.31	106.48	113.12
1	D	194	ILE	N-CA-C	5.28	115.49	110.42
1	B	171	LYS	N-CA-C	-5.25	100.61	109.07
1	B	241	ASP	N-CA-C	-5.22	98.51	108.17
1	C	177	ARG	CD-NE-CZ	-5.16	117.17	124.40
1	D	193	ASP	N-CA-C	-5.15	103.73	110.53
1	C	140	ARG	CD-NE-CZ	-5.14	117.20	124.40
1	A	136	THR	N-CA-C	-5.12	106.37	113.18
1	C	93	VAL	N-CA-C	5.12	115.67	108.36
1	B	140	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	D	260	ASP	N-CA-C	-5.07	106.51	113.30
1	B	194	ILE	N-CA-C	5.06	115.68	110.36
1	C	283	PRO	N-CA-C	5.04	119.28	112.48
1	C	40	ILE	N-CA-C	5.04	116.36	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2683	0	2804	76	0
1	B	2683	0	2804	48	0
1	C	2683	0	2804	105	0
1	D	2683	0	2804	67	0
2	A	254	0	0	14	0
2	B	299	0	0	10	0
2	C	218	0	0	18	0
2	D	259	0	0	17	0
All	All	11762	0	11216	280	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 13.

All (280) 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:8:LEU:HD12	1:A:48:VAL:HG12	1.49	0.93
1:C:246:THR:O	1:C:250:LYS:HG3	1.72	0.90
1:C:221:GLU:O	1:C:224:LYS:HG2	1.72	0.89
1:B:56:ARG:HH11	1:B:56:ARG:HB3	1.39	0.86
1:D:125:ARG:HG3	1:D:127:GLU:HG3	1.58	0.86
1:B:121:LYS:HE3	2:B:387:HOH:O	1.74	0.85
1:C:121:LYS:HZ2	1:D:121:LYS:HG3	1.43	0.84
1:C:253:LYS:HE3	2:C:433:HOH:O	1.77	0.84
1:B:221:GLU:O	1:B:224:LYS:HG2	1.78	0.84
1:C:186:GLU:HG3	2:C:530:HOH:O	1.77	0.83
1:C:218:ILE:HB	1:C:240:VAL:HG12	1.59	0.83
1:A:243:LYS:HE3	1:A:243:LYS:HA	1.59	0.83
1:A:192:MET:HE3	1:A:196:GLU:HG2	1.62	0.82
1:A:247:GLU:OE2	1:A:250:LYS:HD2	1.82	0.80
1:C:195:ASP:O	1:C:199:GLU:HG2	1.83	0.79
1:A:34:GLU:HA	1:A:37:LYS:HE2	1.65	0.78
1:A:175:TRP:HH2	1:A:177:ARG:HE	1.31	0.78
1:C:194:ILE:HD13	1:C:217:ILE:HD11	1.66	0.77
1:C:212:ARG:HG3	2:C:352:HOH:O	1.85	0.76
1:A:121:LYS:HE3	2:A:422:HOH:O	1.85	0.76
1:B:2:ARG:HB3	1:B:3:PRO:HD3	1.68	0.74
1:B:309:ARG:HG2	1:B:333:LEU:HB2	1.69	0.74
1:C:34:GLU:HG2	2:C:522:HOH:O	1.86	0.74
1:C:265:GLU:HG3	2:C:540:HOH:O	1.86	0.74
1:B:48:VAL:CG2	1:B:52:THR:HB	2.18	0.72
1:C:291:GLU:HB2	2:C:484:HOH:O	1.89	0.72
1:C:181:VAL:HG12	2:C:507:HOH:O	1.88	0.72
1:D:181:VAL:O	1:D:185:LYS:HG2	1.90	0.72
1:D:117:HIS:O	1:D:121:LYS:HD2	1.90	0.71
1:C:55:THR:OG1	1:C:57:GLU:HG2	1.91	0.71
1:A:1:MET:HB3	1:A:24:ASP:OD1	1.91	0.70
1:A:247:GLU:HG3	1:A:251:GLN:HE21	1.58	0.69
1:D:264:LYS:NZ	2:D:424:HOH:O	2.25	0.69
1:C:148:LYS:HG2	1:C:171:LYS:HD2	1.73	0.69
1:C:33:GLY:O	1:C:37:LYS:HG3	1.93	0.68
1:D:212:ARG:HG2	2:D:591:HOH:O	1.94	0.67
1:C:121:LYS:HG3	1:D:121:LYS:HZ2	1.60	0.67
1:C:221:GLU:HG2	1:C:224:LYS:HE3	1.77	0.66
1:C:1:MET:HB3	1:C:24:ASP:N	2.10	0.66
1:D:2:ARG:HB3	1:D:3:PRO:HD3	1.76	0.66
1:D:139:LYS:NZ	2:D:514:HOH:O	2.29	0.66
1:C:268:ARG:HB2	1:C:269:GLU:OE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HA	1:A:229:LYS:HD2	1.78	0.65
1:A:188:LYS:HE2	1:A:188:LYS:HA	1.78	0.65
1:D:283:PRO:HD2	1:D:285:TYR:CE2	2.32	0.65
1:A:32:SER:OG	1:A:35:GLU:HG3	1.98	0.64
1:C:288:LEU:HD11	1:D:139:LYS:HD3	1.80	0.64
1:B:319:LYS:NZ	2:B:487:HOH:O	2.30	0.64
1:C:198:LEU:HD22	1:C:226:LEU:HD21	1.78	0.64
1:D:283:PRO:HD2	1:D:285:TYR:CD2	2.33	0.64
1:A:56:ARG:O	1:A:60:GLU:HG2	1.98	0.64
1:C:111:ASN:ND2	1:C:116:ILE:HB	2.13	0.63
1:C:192:MET:HE3	1:C:196:GLU:HG2	1.82	0.61
1:C:309:ARG:HG2	1:C:333:LEU:HB2	1.82	0.61
1:D:49:SER:OG	1:D:51:THR:HG22	2.00	0.61
1:D:219:ASN:O	1:D:223:VAL:HG23	2.01	0.61
1:C:140:ARG:HD3	1:D:290:LEU:HD21	1.82	0.61
1:A:34:GLU:HA	1:A:37:LYS:CE	2.30	0.61
1:C:4:LYS:NZ	2:C:487:HOH:O	2.34	0.61
1:C:192:MET:CE	1:C:200:LYS:HD2	2.32	0.60
1:B:138:PHE:HD1	1:B:138:PHE:O	1.85	0.60
1:B:56:ARG:HH11	1:B:56:ARG:CB	2.11	0.60
1:C:219:ASN:O	1:C:223:VAL:HG23	2.02	0.60
1:B:1:MET:N	2:B:363:HOH:O	2.35	0.59
1:D:299:ARG:HD3	2:D:486:HOH:O	2.02	0.59
1:D:135:TRP:O	1:D:139:LYS:HG2	2.02	0.59
1:A:1:MET:HA	1:A:23:ALA:HA	1.84	0.58
1:A:4:LYS:HD2	2:A:566:HOH:O	2.03	0.58
1:B:178:HIS:O	1:B:180:LYS:HD2	2.03	0.58
1:D:138:PHE:O	1:D:141:ILE:HG13	2.02	0.58
1:A:33:GLY:O	1:A:37:LYS:HG3	2.03	0.58
1:A:288:LEU:HD13	1:B:135:TRP:CE3	2.39	0.58
1:A:293:GLN:HG3	1:B:139:LYS:HE2	1.86	0.58
1:B:1:MET:SD	1:B:23:ALA:C	2.86	0.58
1:C:178:HIS:O	1:C:180:LYS:HD2	2.03	0.58
1:C:217:ILE:HG23	1:C:218:ILE:HG12	1.85	0.58
1:A:288:LEU:HD11	1:B:139:LYS:HG3	1.86	0.57
1:C:87:GLY:HA2	1:C:321:VAL:HG12	1.86	0.56
1:C:139:LYS:O	1:C:139:LYS:HG2	2.04	0.56
1:A:333:LEU:OXT	2:A:562:HOH:O	2.17	0.56
1:C:318:ASN:O	1:C:321:VAL:HG22	2.05	0.56
1:C:57:GLU:HG3	2:C:345:HOH:O	2.06	0.56
1:C:48:VAL:CG2	1:C:52:THR:HB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:GLU:HG3	2:D:390:HOH:O	2.05	0.56
1:A:177:ARG:HH22	1:A:213:ASP:HB3	1.71	0.55
1:D:4:LYS:HD3	2:D:570:HOH:O	2.05	0.55
1:A:292:ALA:O	1:A:296:VAL:HG23	2.05	0.55
1:D:14:GLU:HG3	2:D:547:HOH:O	2.07	0.55
1:C:48:VAL:HG23	1:C:52:THR:HB	1.89	0.55
1:C:121:LYS:NZ	1:D:121:LYS:HG3	2.16	0.55
1:C:14:GLU:CD	1:C:14:GLU:H	2.15	0.55
1:C:309:ARG:HD3	2:C:335:HOH:O	2.07	0.55
1:B:14:GLU:CD	1:B:14:GLU:H	2.15	0.54
1:B:138:PHE:HB2	1:B:277:TRP:CH2	2.42	0.54
1:C:228:GLY:HA2	1:C:255:LYS:HG3	1.89	0.54
1:B:247:GLU:HA	1:B:250:LYS:HG2	1.90	0.54
1:D:298:PHE:O	1:D:302:GLU:HG3	2.07	0.54
1:C:133:LYS:O	1:C:137:GLY:HA3	2.05	0.54
1:C:64:ARG:NH1	2:C:421:HOH:O	2.40	0.54
1:A:247:GLU:HG3	1:A:251:GLN:NE2	2.23	0.53
1:A:291:GLU:HB2	2:A:420:HOH:O	2.09	0.53
1:C:188:LYS:O	1:C:188:LYS:HG2	2.08	0.53
1:D:320:GLU:H	1:D:320:GLU:CD	2.17	0.53
1:C:11:MET:HE3	1:C:71:HIS:HD2	1.74	0.53
1:C:266:PRO:HG2	1:D:130:SER:HA	1.91	0.53
1:A:56:ARG:HG2	1:A:56:ARG:HH11	1.73	0.53
1:C:87:GLY:O	1:C:325:ARG:HD2	2.09	0.53
1:A:197:LEU:HD23	1:A:197:LEU:C	2.34	0.53
1:A:1:MET:HA	1:A:23:ALA:CA	2.38	0.52
1:A:57:GLU:HG3	2:A:417:HOH:O	2.09	0.52
1:D:194:ILE:HD13	1:D:217:ILE:HD11	1.91	0.52
1:B:212:ARG:NH1	2:B:545:HOH:O	2.42	0.52
1:C:138:PHE:HB3	2:C:501:HOH:O	2.09	0.52
1:D:309:ARG:HG3	1:D:333:LEU:HD12	1.91	0.52
1:B:11:MET:HE3	1:B:71:HIS:CD2	2.45	0.51
1:B:41:GLY:O	1:B:64:ARG:HD3	2.11	0.51
1:D:139:LYS:HG3	2:D:435:HOH:O	2.09	0.51
1:B:11:MET:HE3	1:B:71:HIS:HD2	1.76	0.51
1:B:274:LYS:NZ	2:B:592:HOH:O	2.21	0.51
1:C:194:ILE:CD1	1:C:217:ILE:HD11	2.40	0.51
1:C:141:ILE:HD11	1:C:277:TRP:CH2	2.46	0.51
1:C:84:THR:HA	1:C:321:VAL:HG13	1.92	0.51
1:D:178:HIS:HB3	1:D:180:LYS:NZ	2.25	0.51
1:C:65:LEU:HD23	1:C:88:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HD11	1:A:317:VAL:CG1	2.42	0.50
1:D:224:LYS:HG2	1:D:225:LYS:N	2.25	0.50
1:A:192:MET:CE	1:A:196:GLU:HG2	2.38	0.50
1:D:180:LYS:HB3	1:D:182:ASN:OD1	2.12	0.50
1:A:177:ARG:HH22	1:A:213:ASP:CB	2.25	0.50
1:B:138:PHE:O	1:B:138:PHE:CD1	2.64	0.50
1:B:48:VAL:HG23	1:B:52:THR:HB	1.91	0.50
1:C:121:LYS:HZ2	1:D:121:LYS:NZ	2.10	0.50
1:C:1:MET:HE3	1:C:20:LYS:O	2.12	0.49
1:D:27:ILE:N	1:D:27:ILE:HD12	2.27	0.49
1:A:121:LYS:O	1:A:125:ARG:HG3	2.12	0.49
1:C:8:LEU:HA	1:C:28:ILE:O	2.11	0.49
1:C:268:ARG:HG2	1:C:268:ARG:HH11	1.77	0.49
1:D:126:GLY:HA2	2:D:371:HOH:O	2.12	0.49
1:A:194:ILE:HD13	1:A:217:ILE:HD11	1.94	0.49
1:B:291:GLU:CD	1:B:291:GLU:H	2.21	0.49
1:C:61:ASN:N	1:C:61:ASN:HD22	2.11	0.49
1:C:190:ARG:HB2	2:C:452:HOH:O	2.13	0.49
1:B:304:LEU:C	1:B:304:LEU:HD23	2.38	0.49
1:C:234:ILE:HD12	1:C:234:ILE:C	2.38	0.49
1:C:291:GLU:CD	1:C:291:GLU:H	2.21	0.49
1:A:183:VAL:HG22	2:A:489:HOH:O	2.13	0.49
1:A:142:GLU:HG2	1:B:290:LEU:HD12	1.94	0.48
1:D:163:ARG:HG2	1:D:187:LEU:HD21	1.95	0.48
1:C:2:ARG:NH1	1:C:2:ARG:HG3	2.28	0.48
1:C:265:GLU:N	2:C:540:HOH:O	2.33	0.48
1:C:121:LYS:NZ	1:D:121:LYS:NZ	2.62	0.48
1:C:2:ARG:HG3	1:C:2:ARG:HH11	1.79	0.48
1:D:221:GLU:O	1:D:224:LYS:HG2	2.13	0.48
1:C:273:PHE:CD2	1:D:124:ARG:HA	2.49	0.48
1:D:1:MET:N	2:D:360:HOH:O	2.40	0.48
1:D:8:LEU:HD12	1:D:48:VAL:HG12	1.95	0.48
1:C:228:GLY:C	1:C:255:LYS:HG3	2.39	0.48
1:C:4:LYS:NZ	1:C:4:LYS:HB2	2.29	0.47
1:C:192:MET:HE2	1:C:197:LEU:N	2.29	0.47
1:D:131:HIS:HA	2:D:552:HOH:O	2.14	0.47
1:C:327:ILE:O	1:C:330:VAL:HG22	2.14	0.47
1:D:184:GLU:O	1:D:188:LYS:HA	2.14	0.47
1:A:175:TRP:HH2	1:A:177:ARG:NE	2.08	0.47
1:A:56:ARG:HG3	1:A:82:GLU:HG2	1.97	0.47
1:B:63:GLU:HG3	2:B:479:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HG3	1:D:24:ASP:OD1	2.14	0.47
1:B:309:ARG:HG2	1:B:333:LEU:CB	2.43	0.47
1:B:247:GLU:OE1	1:B:250:LYS:HD2	2.14	0.47
1:C:122:PHE:CZ	1:C:127:GLU:HB3	2.50	0.47
1:C:218:ILE:CB	1:C:240:VAL:HG12	2.38	0.47
1:A:132:ALA:O	1:A:136:THR:HB	2.15	0.46
1:C:292:ALA:O	1:C:296:VAL:HG23	2.15	0.46
1:D:1:MET:HE1	1:D:21:LYS:C	2.41	0.46
1:A:195:ASP:O	1:A:199:GLU:HG3	2.15	0.46
1:A:247:GLU:HA	1:A:250:LYS:HG2	1.97	0.46
1:C:2:ARG:N	1:C:3:PRO:HD2	2.31	0.46
1:D:1:MET:HE2	2:D:566:HOH:O	2.15	0.46
1:D:13:ARG:HD2	2:D:469:HOH:O	2.15	0.46
1:D:123:ILE:HG23	1:D:124:ARG:N	2.31	0.46
1:C:11:MET:HE3	1:C:71:HIS:CD2	2.51	0.46
1:C:165:LEU:O	1:C:168:PHE:HB2	2.16	0.46
1:C:73:ALA:O	1:C:92:LYS:HD2	2.15	0.46
1:D:204:VAL:HG21	1:D:226:LEU:HD21	1.98	0.46
1:A:177:ARG:HD3	2:A:537:HOH:O	2.15	0.46
1:C:39:VAL:O	1:C:42:ARG:HG2	2.15	0.46
1:C:135:TRP:HA	1:D:288:LEU:HD22	1.98	0.46
1:A:177:ARG:HH11	1:A:177:ARG:HG2	1.81	0.46
1:B:48:VAL:HG22	1:B:49:SER:N	2.31	0.45
1:C:325:ARG:HD3	1:C:330:VAL:CG1	2.46	0.45
1:D:39:VAL:HG12	1:D:42:ARG:NH2	2.31	0.45
1:C:192:MET:HE3	1:C:200:LYS:HD2	1.97	0.45
1:A:234:ILE:HD12	1:A:234:ILE:C	2.41	0.45
1:A:55:THR:OG1	1:A:58:VAL:HG23	2.15	0.45
1:B:253:LYS:HD3	2:B:585:HOH:O	2.17	0.45
1:D:260:ASP:CG	1:D:284:HIS:HA	2.41	0.45
1:C:192:MET:CE	1:C:197:LEU:HA	2.47	0.45
1:D:85:LYS:NZ	2:D:410:HOH:O	2.41	0.45
1:B:1:MET:SD	1:B:23:ALA:O	2.75	0.45
1:C:1:MET:HB3	1:C:23:ALA:C	2.42	0.45
1:A:159:LYS:O	1:A:163:ARG:HG3	2.16	0.45
1:B:260:ASP:CG	1:B:284:HIS:HA	2.42	0.45
1:D:304:LEU:C	1:D:304:LEU:HD23	2.41	0.45
1:C:27:ILE:HD13	2:C:338:HOH:O	2.18	0.44
1:D:197:LEU:C	1:D:197:LEU:HD23	2.43	0.44
1:A:171:LYS:NZ	1:A:171:LYS:HB3	2.32	0.44
1:A:8:LEU:HA	1:A:28:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:PRO:HG2	1:C:23:ALA:HB2	2.00	0.44
1:C:206:LEU:HB2	1:C:233:ASN:HA	1.99	0.44
1:A:46:ILE:HD12	1:A:48:VAL:CG1	2.48	0.44
1:A:80:LEU:HD11	1:A:317:VAL:HG12	1.98	0.44
1:C:2:ARG:HB3	1:C:3:PRO:HD3	2.00	0.44
1:D:109:ILE:O	1:D:113:MET:HG2	2.17	0.44
1:A:53:LYS:NZ	2:A:463:HOH:O	2.50	0.44
1:C:185:LYS:HB3	2:C:530:HOH:O	2.18	0.44
1:D:2:ARG:HG2	2:D:407:HOH:O	2.18	0.44
1:A:2:ARG:NH1	1:A:2:ARG:HG3	2.33	0.44
1:B:319:LYS:CE	2:B:487:HOH:O	2.66	0.44
1:C:162:ALA:HB1	1:C:187:LEU:HD13	1.99	0.43
1:C:206:LEU:HD11	1:C:240:VAL:CG1	2.49	0.43
1:B:152:LEU:HD12	1:B:206:LEU:CD2	2.48	0.43
1:D:121:LYS:O	1:D:125:ARG:HG2	2.18	0.43
1:D:159:LYS:O	1:D:163:ARG:HG3	2.17	0.43
1:A:1:MET:HE2	1:A:24:ASP:HA	2.00	0.43
1:C:13:ARG:NH2	1:C:14:GLU:OE2	2.52	0.43
1:A:174:TYR:HE2	1:A:184:GLU:HG2	1.83	0.43
1:B:138:PHE:HA	2:B:367:HOH:O	2.17	0.43
1:B:260:ASP:O	1:B:284:HIS:HA	2.19	0.43
1:A:192:MET:CE	1:A:200:LYS:HD2	2.48	0.43
1:D:89:TYR:OH	1:D:322:LEU:HD23	2.19	0.43
1:D:105:THR:HG21	1:D:161:ILE:HD13	2.01	0.43
1:A:188:LYS:HA	1:A:188:LYS:CE	2.45	0.43
1:B:320:GLU:H	1:B:320:GLU:CD	2.26	0.43
1:A:171:LYS:NZ	2:A:580:HOH:O	2.24	0.42
1:B:56:ARG:NH1	1:B:57:GLU:N	2.67	0.42
1:C:82:GLU:OE2	1:C:85:LYS:HE3	2.18	0.42
1:B:319:LYS:HE2	2:B:487:HOH:O	2.19	0.42
1:C:180:LYS:O	1:C:184:GLU:HG3	2.20	0.42
1:A:177:ARG:NH1	2:A:462:HOH:O	2.49	0.42
1:B:197:LEU:C	1:B:197:LEU:HD23	2.45	0.42
1:C:228:GLY:CA	1:C:255:LYS:HG3	2.50	0.42
1:A:37:LYS:HD3	1:A:57:GLU:HG2	2.01	0.42
1:C:121:LYS:NZ	1:D:121:LYS:HZ2	2.18	0.42
1:A:2:ARG:C	1:A:2:ARG:HD2	2.44	0.42
1:A:253:LYS:HD2	2:A:446:HOH:O	2.19	0.42
1:A:175:TRP:CH2	1:A:177:ARG:NE	2.84	0.42
1:B:14:GLU:CD	1:B:14:GLU:N	2.77	0.42
1:C:2:ARG:HB3	1:C:3:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:PHE:HB2	1:B:277:TRP:HH2	1.84	0.42
1:C:150:GLY:HA2	1:C:173:TYR:O	2.19	0.42
1:D:154:MET:HG2	1:D:183:VAL:HG11	2.01	0.42
1:A:140:ARG:NH2	2:A:464:HOH:O	2.52	0.41
1:A:217:ILE:HG23	1:A:218:ILE:HG12	2.02	0.41
1:A:246:THR:HA	1:A:272:LEU:HD21	2.02	0.41
1:B:194:ILE:HD13	1:B:217:ILE:HD11	2.02	0.41
1:A:265:GLU:HG2	1:B:128:TRP:CH2	2.55	0.41
1:C:53:LYS:NZ	2:C:390:HOH:O	2.35	0.41
1:D:96:LEU:HD12	1:D:295:ASP:HB2	2.02	0.41
1:A:7:VAL:HG23	1:A:25:VAL:HG13	2.02	0.41
1:A:155:GLY:O	1:A:159:LYS:HG3	2.20	0.41
1:C:56:ARG:HG2	1:C:56:ARG:HH11	1.86	0.41
1:D:9:LEU:HD11	1:D:71:HIS:CG	2.55	0.41
1:A:133:LYS:O	1:A:137:GLY:HA3	2.21	0.41
1:C:61:ASN:N	1:C:61:ASN:ND2	2.68	0.41
1:C:162:ALA:CB	1:C:187:LEU:HD13	2.51	0.41
1:A:180:LYS:O	1:A:184:GLU:HG3	2.21	0.41
1:A:264:LYS:HE2	2:A:468:HOH:O	2.19	0.41
1:C:53:LYS:HE3	2:C:431:HOH:O	2.20	0.41
1:C:192:MET:HE2	1:C:197:LEU:HA	2.03	0.41
1:C:291:GLU:HB2	2:D:382:HOH:O	2.20	0.41
1:A:2:ARG:NH2	1:A:332:MET:O	2.49	0.41
1:B:201:SER:O	1:B:229:LYS:HD3	2.20	0.40
1:C:187:LEU:O	1:C:188:LYS:HB3	2.21	0.40
1:C:111:ASN:HD22	1:C:116:ILE:HB	1.84	0.40
1:A:291:GLU:CD	1:A:291:GLU:H	2.30	0.40
1:A:299:ARG:HD3	1:A:299:ARG:HA	1.82	0.40
1:D:162:ALA:O	1:D:166:ILE:HG13	2.22	0.40
1:A:62:ALA:HB1	1:A:65:LEU:CB	2.52	0.40
1:A:252:GLY:HA2	2:A:467:HOH:O	2.21	0.40
1:D:55:THR:HB	2:D:354:HOH:O	2.21	0.40
1:D:135:TRP:CD1	1:D:135:TRP:N	2.90	0.40

There are no symmetry-related clashes.

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	331/333 (99%)	314 (95%)	16 (5%)	1 (0%)	36	28
1	B	331/333 (99%)	315 (95%)	15 (4%)	1 (0%)	36	28
1	C	331/333 (99%)	311 (94%)	19 (6%)	1 (0%)	36	28
1	D	331/333 (99%)	317 (96%)	12 (4%)	2 (1%)	21	12
All	All	1324/1332 (99%)	1257 (95%)	62 (5%)	5 (0%)	30	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	290	LEU
1	D	140	ARG
1	A	194	ILE
1	B	2	ARG
1	C	183	VAL

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	286/286 (100%)	283 (99%)	3 (1%)	68	67
1	B	286/286 (100%)	283 (99%)	3 (1%)	68	67
1	C	286/286 (100%)	280 (98%)	6 (2%)	47	41
1	D	286/286 (100%)	278 (97%)	8 (3%)	38	30
All	All	1144/1144 (100%)	1124 (98%)	20 (2%)	53	49

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	LYS
1	A	299	ARG
1	A	320	GLU
1	B	1	MET
1	B	56	ARG
1	B	186	GLU
1	C	4	LYS
1	C	61	ASN
1	C	80	LEU
1	C	111	ASN
1	C	321	VAL
1	C	328	GLU
1	D	4	LYS
1	D	16	LEU
1	D	94	SER
1	D	139	LYS
1	D	141	ILE
1	D	185	LYS
1	D	186	GLU
1	D	291	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	251	GLN
1	A	329	ASN
1	B	178	HIS
1	C	61	ASN
1	C	71	HIS
1	C	111	ASN
1	C	329	ASN
1	D	111	ASN
1	D	131	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	333/333 (100%)	0.61	18 (5%) 31 37	15, 27, 47, 71	0
1	B	333/333 (100%)	0.46	16 (4%) 35 41	16, 25, 41, 56	0
1	C	333/333 (100%)	1.21	65 (19%) 3 3	20, 34, 58, 73	0
1	D	333/333 (100%)	0.64	21 (6%) 26 30	19, 28, 44, 54	0
All	All	1332/1332 (100%)	0.73	120 (9%) 15 17	15, 29, 50, 73	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	7.0
1	B	138	PHE	6.8
1	C	1	MET	5.6
1	D	183	VAL	5.4
1	A	1	MET	5.4
1	C	187	LEU	4.6
1	A	187	LEU	4.1
1	D	138	PHE	3.9
1	D	185	LYS	3.9
1	D	182	ASN	3.8
1	C	211	THR	3.7
1	B	292	ALA	3.7
1	C	272	LEU	3.6
1	D	181	VAL	3.5
1	A	193	ASP	3.4
1	C	226	LEU	3.4
1	C	138	PHE	3.4
1	C	181	VAL	3.3
1	C	267	VAL	3.3
1	C	189	ALA	3.3
1	C	275	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	135	TRP	3.3
1	D	292	ALA	3.3
1	A	183	VAL	3.2
1	C	191	TYR	3.1
1	C	198	LEU	3.1
1	C	192	MET	3.1
1	C	238	ALA	3.0
1	C	140	ARG	3.0
1	D	1	MET	3.0
1	A	177	ARG	3.0
1	C	197	LEU	2.9
1	B	317	VAL	2.9
1	A	178	HIS	2.9
1	C	302	GLU	2.9
1	C	194	ILE	2.9
1	D	178	HIS	2.8
1	A	181	VAL	2.8
1	C	183	VAL	2.8
1	D	139	LYS	2.8
1	C	141	ILE	2.8
1	D	135	TRP	2.8
1	C	135	TRP	2.8
1	C	118	TYR	2.7
1	C	244	ALA	2.7
1	C	268	ARG	2.7
1	B	291	GLU	2.7
1	C	149	VAL	2.7
1	C	327	ILE	2.7
1	D	2	ARG	2.7
1	A	185	LYS	2.7
1	D	186	GLU	2.7
1	C	175	TRP	2.7
1	B	137	GLY	2.6
1	A	191	TYR	2.6
1	C	196	GLU	2.6
1	D	294	GLU	2.6
1	C	80	LEU	2.6
1	A	2	ARG	2.6
1	B	139	LYS	2.6
1	C	251	GLN	2.6
1	C	223	VAL	2.6
1	D	132	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	218	ILE	2.6
1	C	269	GLU	2.6
1	C	182	ASN	2.6
1	C	214	THR	2.6
1	C	134	ILE	2.5
1	D	119	ALA	2.5
1	C	215	TYR	2.5
1	D	131	HIS	2.5
1	C	250	LYS	2.5
1	D	123	ILE	2.5
1	C	324	VAL	2.5
1	B	185	LYS	2.5
1	C	177	ARG	2.4
1	B	187	LEU	2.4
1	C	193	ASP	2.4
1	A	140	ARG	2.4
1	A	63	GLU	2.4
1	C	273	PHE	2.4
1	C	195	ASP	2.4
1	A	25	VAL	2.4
1	B	182	ASN	2.4
1	C	176	SER	2.4
1	C	326	PRO	2.4
1	B	333	LEU	2.3
1	B	84	THR	2.3
1	D	322	LEU	2.3
1	B	2	ARG	2.3
1	C	2	ARG	2.3
1	C	153	GLY	2.3
1	C	203	ILE	2.3
1	C	186	GLU	2.3
1	D	63	GLU	2.3
1	C	224	LYS	2.3
1	C	234	ILE	2.2
1	C	212	ARG	2.2
1	C	94	SER	2.2
1	C	262	PHE	2.2
1	A	223	VAL	2.2
1	C	213	ASP	2.2
1	D	130	SER	2.2
1	C	139	LYS	2.2
1	C	312	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	226	LEU	2.1
1	A	192	MET	2.1
1	C	199	GLU	2.1
1	A	199	GLU	2.1
1	C	178	HIS	2.1
1	B	189	ALA	2.1
1	C	132	ALA	2.1
1	A	328	GLU	2.1
1	C	180	LYS	2.0
1	C	266	PRO	2.0
1	A	80	LEU	2.0
1	C	119	ALA	2.0
1	B	136	THR	2.0
1	C	228	GLY	2.0
1	C	240	VAL	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.